STN SEARCH TRANSCRIPT 10/772,235

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PASSWORD:
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 NEWS  1          Web Page URLs for STN Seminar Schedule - N. America
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 NEWS 18  DEC 27  CA/CAplus enhanced with more pre-1907 records
 NEWS 19  JAN 08  CHEMLIST enhanced with New Zealand Inventory of Chemicals
 NEWS 20  JAN 16  CA/CAplus Company Name Thesaurus enhanced and reloaded
 NEWS 21  JAN 16  IPC version 2007.01 thesaurus available on STN
 NEWS 22  JAN 16  WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data

 NEWS EXPRESS  NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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 NEWS IPC8     For general information regarding STN implementation of IPC 8
 NEWS X25      X.25 communication option no longer available

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FILE 'HOME' ENTERED AT 09:06:06 ON 22 JAN 2007

=> FILE REG
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY     SESSION
FULL ESTIMATED COST                                    0.21        0.21

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DICTIONARY FILE UPDATES:  21 JAN 2007  HIGHEST RN 917948-20-0

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http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\LI and ZHANG DIV.str
```

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chain nodes :
19
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  22
chain bonds :
3-19
ring bonds :
1-2  1-6  1-7  2-3  2-10  3-4  4-5  5-6  6-11  7-8  7-22  8-9  9-10  11-12  11-13
12-16  12-22  13-14  14-15  15-16
exact/norm bonds :
1-2  1-6  1-7  2-3  3-4  3-19  4-5  5-6  6-11  7-8  7-22  11-12  11-13  12-16
12-22
normalized bonds :
2-10  8-9  9-10  13-14  14-15  15-16
isolated ring systems :
containing 1 :

G1:O,S,N

G2:O,S

G3:C,O,S,N

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  19:CLASS  22:CLASS


L1      STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1             STR
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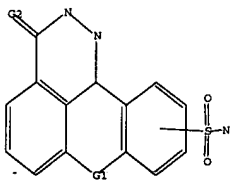

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G1 O,S,N
G2 O,S


Structure attributes must be viewed using STN Express query preparation.

=> S L1
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SAMPLE SCREEN SEARCH COMPLETED -        0 TO ITERATE

100.0% PROCESSED         0 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            0 TO        0
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> S L1 SSS FULL
FULL SEARCH INITIATED 09:16:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -        13 TO ITERATE

100.0% PROCESSED       13 ITERATIONS                                8 ANSWERS
SEARCH TIME: 00.00.01

L3            8 SEA SSS FUL L1

=> FILE CAPLUS
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY     SESSION
FULL ESTIMATED COST                                  178.40      178.61

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FILE COVERS 1907 - 22 Jan 2007  VOL 146 ISS 5
FILE LAST UPDATED: 21 Jan 2007  (20070121/ED)

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=> S L3
L4             1 L3

=> D

L4   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2007 ACS on STN
AN   2001:167996  CAPLUS
DN   134:207821
TI   Preparation of [1]benzopyrano[4,3,2-de]phthalazine-3(2H)-ones,
     pharmaceutical compositions and use for treating cellular damage, such as
     neural or cardiovascular tissue damage
IN   Li, Jia-He; Zhang, Jie
PA   Guilford Pharmaceuticals Inc., USA
SO   PCT Int. Appl., 95 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ----------          ----   --------    --------------------   --------
PI   WO 2001016137       A1     20010308    WO 2000-US23745        20000830
        W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
            HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
            LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
            SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
            YU, ZA, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
            DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
            CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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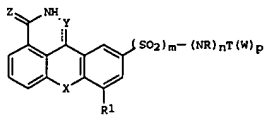
US 6291425	B1	20010918	US 1999-387767	19990901
CA 2382317	A1	20010308	CA 2000-2382317	20000830
EP 1212328	A1	20020612	EP 2000-959578	20000830
EP 1212328	B1	20060802		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003508400	T	20030304	JP 2001-519703	20000830
AT 334985	T	20060815	AT 2000-959578	20000830
US 6716828	B1	20040406	US 2001-781195	20010213
US 2005074470	A1	20050407	US 2004-772235	20040206
AU 2005202592	A1	20050707	AU 2005-202592	20050615
PRAI US 1999-387767	A	19990901		
WO 2000-US23745	W	20000830		
US 2001-781195	A3	20010213		

OS MARPAT 134:207821
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> D ABS HITSTR

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
GI



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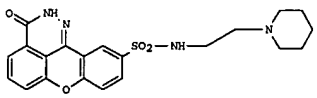
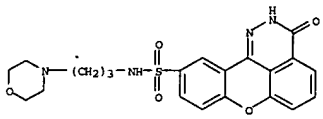


II

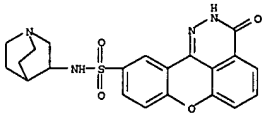
AB Title compds. [I; R = H, lower alkyl; R1 = H, SO3H; m = 0, 1; n = 0, 1; p = 1, 2; Y = CO, O, N; Z = O, S; X = O, S, bond; W = CN, heteoaryl, cycloalkyl; COCH3, SO3H, H; T = alkenylene, arylene, aralkylene, alkarylene, bond; dotted = single, double], pharmaceutically acceptable salt, hydrate, and prodrug are prepared as PARP inhibitors in pharmaceutical compns., and methods of using the disclosed compds. for treating cellular damage, such as neural or cardiovascular tissue damages. Thus, the title compound II was prepared

IT 328525-75-3P 328526-08-5P 328526-21-2P
328526-27-8P 328526-28-9P 328526-33-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzopyranodephthalazineonesas PARP inhibitors for treating cellular damages)

RN 328525-75-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-3-oxo-N-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

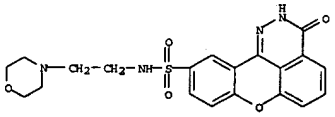


RN 328526-33-6 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,N-1-azabicyclo[2.2.2]oct-3-yl-2,3-dihydro-3-oxo-(9CI) (CA INDEX NAME)



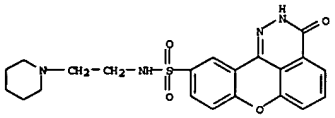
IT 328525-96-8P 328525-97-9P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzopyranodephthalazineonesas PARP inhibitors for treating cellular damages)

RN 328525-96-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-N-[2-(4-morpholinyl)ethyl]-3-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

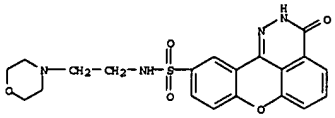


● HCl

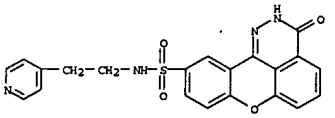
RN 328525-97-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-3-oxo-N-[2-(1-piperidinyl)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



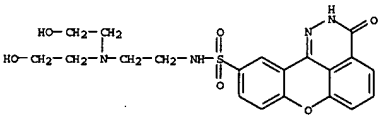
RN 328526-08-5 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-N-[2-(4-morpholinyl)ethyl]-3-oxo- (9CI) (CA INDEX NAME)



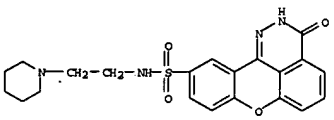
RN 328526-21-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-3-oxo-N-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



RN 328526-27-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,N-[2-[bis(2-hydroxyethyl)amino]ethyl]-2,3-dihydro-3-oxo-(9CI) (CA INDEX NAME)



RN 328526-28-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-N-[3-(4-morpholinyl)propyl]-3-oxo- (9CI) (CA INDEX NAME)



● HCl

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LOGOFF? (Y)/N/HOLD:Y

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.78	-0.78

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                functionality
NEWS 14  DEC 18  CA/CAplus pre-1967 chemical substance index entries enhanced
                with preparation role
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                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'MEDLINE' ENTERED AT 09:26:23 ON 22 JAN 2007

 FILE LAST UPDATED: 20 Jan 2007 (20070120/UP).  FILE COVERS 1950 TO DATE.

  All regular MEDLINE updates from November 15 to December 16 have been
  added to MEDLINE, along with 2007 Medical Subject Headings (MeSH(R))
  and 2007 tree numbers.

  The annual reload will be available in early 2007.

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

=> S PARP AND INHIBIT?
         3230 PARP
           60 PARPS
         3236 PARP
                (PARP OR PARPS)
      1307865 INHIBIT?
L1       2215 PARP AND INHIBIT?

=> S L1 AND (THERAPY OR THERAPEUTIC OR CLINICAL)
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        72832 THERAPIES
      2572636 THERAPY
                (THERAPY OR THERAPIES)
      1520912 THERAPEUTIC
        19287 THERAPEUTICS
      1534336 THERAPEUTIC
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      1513357 CLINICAL
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L2         731 L1 AND (THERAPY OR THERAPEUTIC OR CLINICAL)

=> S L2 AND REVIEW
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        58448 REVIEWS
       511397 REVIEW
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L3          22 L2 AND REVIEW

=> S L3 AND 1999/PY
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L4           1 L3 AND 1999/PY

=> D

L4   ANSWER 1 OF 1      MEDLINE on STN
AN   2005453539      MEDLINE
DN   PubMed ID: 16121295
TI   A novel PARP inhibitor, ion channel modulation and AD
     therapies.
AU   Worker C
CS   Current Drugs Ltd, Middlesex House, 34-42 Cleveland Street, London, W1P
     6LB, UK.. charlotte@cursci.co.uk
SO   IDrugs : the investigational drugs journal, (1999 Sep) Vol. 2,
     No. 9, pp. 859-60.
     Journal code: 100883655. ISSN: 1369-7056.
CY   England: United Kingdom
DT   Journal; Article; (JOURNAL ARTICLE)
LA   English
FS   NONMEDLINE; PUBMED-NOT-MEDLINE
EM   200510
ED   Entered STN: 26 Aug 2005
     Last Updated on STN: 14 Oct 2005
     Entered Medline: 13 Oct 2005

=> D ABS

L4   ANSWER 1 OF 1      MEDLINE on STN
AB   On the fourth and final day of the EPHAR congress, ion channel modulation
     was the topic for two symposia and plenary lectures.  The potential of
     dual potassium and calcium channel blockers as antiarrhythmics was
     discussed, amongst other applications for ion channel modifiers.  Several
     presentations were dedicated to the disclosure of a novel PARP
     inhibitor, BGP15, developed at the University Medical School of
     Pecs in Hungary.  This compound is emerging as a promising potential
     anti-ischemic and a chemoprotective agent.  The treatment of Alzheimer's
     disease (AD) was the subject of further discussions; a detailed
     presentation was given by a psychiatrist from the US, describing the
     treatment regimens favored in her clinic, as well as a complete
     review of currently available and potentially new AD
     therapies.

=> LOGOFF

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:Y
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       1.39       1.60

STN INTERNATIONAL LOGOFF AT 09:28:06 ON 22 JAN 2007


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                to 50,000
NEWS 10  DEC 01  CAS REGISTRY updated with new ambiguity codes
NEWS 11  DEC 11  CAS REGISTRY chemical nomenclature enhanced
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NEWS 13  DEC 14  GBFULL and FRFULL enhanced with IPC 8 features and
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NEWS 14  DEC 18  CA/CAplus pre-1967 chemical substance index entries enhanced
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NEWS 15  DEC 18  CA/CAplus patent kind codes updated
NEWS 16  DEC 18  MARPAT to CA/CAplus accession number crossover limit increased
                to 50,000
NEWS 17  DEC 18  MEDLINE updated in preparation for 2007 reload
NEWS 18  DEC 27  CA/CAplus enhanced with more pre-1907 records
NEWS 19  JAN 08  CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 20  JAN 16  CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 21  JAN 16  IPC version 2007.01 thesaurus available on STN
NEWS 22  JAN 16  WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data

NEWS EXPRESS  NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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FILE 'HOME' ENTERED AT 09:31:32 ON 22 JAN 2007

=> FILE MEDLINE
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'MEDLINE' ENTERED AT 09:31:38 ON 22 JAN 2007

 FILE LAST UPDATED: 20 Jan 2007 (20070120/UP).  FILE COVERS 1950 TO DATE.

  All regular MEDLINE updates from November 15 to December 16 have been
  added to MEDLINE, along with 2007 Medical Subject Headings (MeSH(R))
  and 2007 tree numbers.

  The annual reload will be available in early 2007.

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

=> S PARP AND INHIBIT?
         3230 PARP
           60 PARPS
         3236 PARP
                (PARP OR PARPS)
      1307865 INHIBIT?
L1       2215 PARP AND INHIBIT?

=> S L1 AND (THERAPY OR THERAPEUTIC OR CLINICAL)
      2547648 THERAPY
        72832 THERAPIES
      2572636 THERAPY
                (THERAPY OR THERAPIES)
      1520912 THERAPEUTIC
        19287 THERAPEUTICS
      1534336 THERAPEUTIC
                (THERAPEUTIC OR THERAPEUTICS)
      1513357 CLINICAL
           48 CLINICALS
      1513384 CLINICAL
                (CLINICAL OR CLINICALS)
L2         731 L1 AND (THERAPY OR THERAPEUTIC OR CLINICAL)

=> S L2 AND REVIEW
       466427 REVIEW
        58448 REVIEWS
       511397 REVIEW
                (REVIEW OR REVIEWS)
L3          22 L2 AND REVIEW

=> S L3 AND 2000/PY
       491374 2000/PY
                (20000000-20009999/PY)
L4           0 L3 AND 2000/PY
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=> S L3 AND 2001/PY
      520788 2001/PY
             (20010000-20019999/PY)
L5            0 L3 AND 2001/PY

=> S L3 AND 2002/PY
      544209 2002/PY
             (20020000-20029999/PY)
L6            2 L3 AND 2002/PY

=> D 1-2 IBIB ABS

L6   ANSWER 1 OF 2     MEDLINE on STN
ACCESSION NUMBER:   2002464432     MEDLINE
DOCUMENT NUMBER:    PubMed ID: 12223530
TITLE:              The therapeutic potential of poly(ADP-ribose)
                    polymerase inhibitors.
AUTHOR:             Virag Laszlo; Szabo Csaba
CORPORATE SOURCE:   Inotek Pharmaceutical Corp., Beverly, Massachusetts 01915,
                    USA.
CONTRACT NUMBER:    R01GM60915 (NIGMS)
SOURCE:             Pharmacological reviews, (2002 Sep) Vol. 54, No.
                    3, pp. 375-429.  Ref: 630
                    Journal code: 0421737. ISSN: 0031-6997.
PUB. COUNTRY:       United States
DOCUMENT TYPE:      Journal; Article; (JOURNAL ARTICLE)
                    General Review; (REVIEW)
LANGUAGE:           English
FILE SEGMENT:       Priority Journals
ENTRY MONTH:        200303
ENTRY DATE:         Entered STN: 12 Sep 2002
                    Last Updated on STN: 11 Mar 2003
                    Entered Medline: 10 Mar 2003
AB  Poly(ADP-ribose) polymerase-1 (PARP-1) is a member of the
    PARP enzyme family consisting of PARP-1 and several
    recently identified novel poly(ADP-ribosylating) enzymes.  PARP
    -1 is an abundant nuclear protein functioning as a DNA nick-sensor enzyme.
    Upon binding to DNA breaks, activated PARP cleaves NAD(+) into
    nicotinamide and ADP-ribose and polymerizes the latter onto nuclear
    acceptor proteins including histones, transcription factors, and
    PARP itself.  Poly(ADP-ribosylation) contributes to DNA repair and
    to the maintenance of genomic stability.  On the other hand, oxidative
    stress-induced overactivation of PARP consumes NAD(+) and
    consequently ATP, culminating in cell dysfunction or necrosis.  This
    cellular suicide mechanism has been implicated in the pathomechanism of
    stroke, myocardial ischemia, diabetes, diabetes-associated cardiovascular
    dysfunction, shock, traumatic central nervous system injury, arthritis,
    colitis, allergic encephalomyelitis, and various other forms of
    inflammation.  PARP has also been shown to associate with and
    regulate the function of several transcription factors.  Of special
    interest is the enhancement by PARP of nuclear factor kappa
    B-mediated transcription, which plays a central role in the expression of
    inflammatory cytokines, chemokines, adhesion molecules, and inflammatory
    mediators.  Herein we review the double-edged sword roles of
    PARP in DNA damage signaling and cell death and summarize the
    underlying mechanisms of the anti-inflammatory effects of PARP
    inhibitors.  Moreover, we discuss the potential use of
    PARP inhibitors as anticancer agents, radiosensitizers,
    and antiviral agents.

L6   ANSWER 2 OF 2     MEDLINE on STN
ACCESSION NUMBER:   2002410571     MEDLINE
DOCUMENT NUMBER:    PubMed ID: 12164482
TITLE:              Modulating poly (ADP-ribose) polymerase activity: potential
                    for the prevention and therapy of pathogenic
                    situations involving DNA damage and oxidative stress.
AUTHOR:             Decker Patrice; Muller Sylviane
CORPORATE SOURCE:   Institute for Cell Biology, Department of Immunology, Auf
                    der Morgenstelle, Tubingen, Germany.. patrice.decker@uni-
                    tuebingen.de
SOURCE:             Current pharmaceutical biotechnology, (2002 Sep)
                    Vol. 3, No. 3, pp. 275-83.  Ref: 100
                    Journal code: 100960530. ISSN: 1389-2010.
PUB. COUNTRY:       Netherlands
DOCUMENT TYPE:      Journal; Article; (JOURNAL ARTICLE)
                    General Review; (REVIEW)
LANGUAGE:           English
FILE SEGMENT:       Priority Journals
ENTRY MONTH:        200302
ENTRY DATE:         Entered STN: 8 Aug 2002
                    Last Updated on STN: 11 Feb 2003
                    Entered Medline: 10 Feb 2003
AB  Poly (ADP-ribose) polymerase is a zinc-finger DNA-binding enzyme which
    detects and signals DNA strand breaks generated either directly during
    base excision repair, or indirectly by genotoxic agents such as oxygen
    radicals.  In response to genotoxic injury, PARP catalyses the
    synthesis of poly (ADP-ribose), from its substrate beta-NAD+ and this
    polymer is covalently attached to several nuclear proteins and
    PARP itself.  As a result, PARP converts DNA breaks into
    intracellular signals which activate DNA repair programs or cell death
    options.  Several studies have also shown that PARP is involved
    in either necrosis and subsequent inflammation or apoptosis.  Although
    this enzyme is not indispensable during the latter cell death program, it
    has been demonstrated that PARP plays a facilitating role in
    this process.  PARP is activated at an intermediate stage of
    apoptosis and is then cleaved and inactivated at a late stage by apoptotic
    proteases, namely caspase-3/CPP-32/Yama/apopain and caspase-7.  This
    cleavage prevents necrosis during apoptosis, avoiding inflammation.  All
    these functions, and the observation that PARP is an abundant
    and highly conserved enzyme, suggest that this enzyme plays a pivotal
    role, particularly in the maintenance of genomic DNA stability, apoptosis
    and in the response to oxidative stress.  Since these situations are found
    in cancer, inflammation, autoimmunity (such as diabetes), myocardial
    dysfunction, certain infections, ageing and radiation/chemical exposure,
    attempts have been made to modulate PARP activity.  With regard
    to the increasing interest towards PARP, the aim of this
    review is to explain the cellular role of PARP and the
    advantages of modulating its activity in diverse preventive or
    therapeutic strategies.


=> S L3 AND 2003/PY
      571736 2003/PY
             (20030000-20039999/PY)
L7            2 L3 AND 2003/PY

=> D 1-2 IBIB ABS

L7   ANSWER 1 OF 2     MEDLINE on STN
ACCESSION NUMBER:   2003467908     MEDLINE
DOCUMENT NUMBER:    PubMed ID: 14529457
TITLE:              Recent developments on the role of mitochondria in
                    poly(ADP-ribose) polymerase inhibition.
AUTHOR:             Klaidman L K; Yang J; Chang M L; Adams J D Jr
CORPORATE SOURCE:   University of Southern California, School of Pharmacy, 1985
                    Zonal Avenue, Los Angeles, CA 90089, USA.
SOURCE:             Current medicinal chemistry, (2003 Dec) Vol. 10,
                    No. 24, pp. 2669-78.  Ref: 106
                    Journal code: 9440157. ISSN: 0929-8673.
PUB. COUNTRY:       Netherlands
DOCUMENT TYPE:      Journal; Article; (JOURNAL ARTICLE)
                    General Review; (REVIEW)
LANGUAGE:           English
FILE SEGMENT:       Priority Journals
ENTRY MONTH:        200402
ENTRY DATE:         Entered STN: 8 Oct 2003
                    Last Updated on STN: 3 Feb 2004
                    Entered Medline: 2 Feb 2004
AB  Numerous pathophysiological disorders involve some element of oxidative
    stress and bioenergetic deficit.  Poly(ADP-ribose) polymerase-1 (
    PARP-1) inhibitors have been used recently as a
    promising new therapeutic strategy aimed at halting the
    bioenergetic decline associated with oxidative brain insults and other
    conditions.  PARP-1 uses NAD+ as a substrate and is activated
    during stressful circumstances, mainly in the nucleus.  PARP-1
    inhibitors are well known for blocking the excessive consumption
    of NAD+, thereby preserving energy metabolism.  But what is the role of
    mitochondria in this process? Recent investigations have begun to focus on
    whether mitochondrial function can also be preserved by PARP-1
    inhibitors.  This review will present some of the latest
    mechanistic evidence documenting the potential involvement of PARP
    -1 inhibitors in protecting mitochondrial function and
    preventing necrosis, apoptosis and mitochondrial calcium cycling.

L7   ANSWER 2 OF 2     MEDLINE on STN
ACCESSION NUMBER:   2003301532     MEDLINE
DOCUMENT NUMBER:    PubMed ID: 12829019
TITLE:              PARP-1, a determinant of cell survival in
                    response to DNA damage.
AUTHOR:             Bouchard Veronique J; Rouleau Michele; Poirier Guy G
CORPORATE SOURCE:   Health and Environment Unit, Faculty of Medicine, Laval
                    University Medical Research Center, 2705 Boulevard Laurier,
                    Ste-Foy, Quebec, Canada G1V 4G2.
SOURCE:             Experimental hematology, (2003 Jun) Vol. 31, No.
                    6, pp. 446-54.  Ref: 111
                    Journal code: 0402313. ISSN: 0301-472X.
PUB. COUNTRY:       Netherlands
DOCUMENT TYPE:      Journal; Article; (JOURNAL ARTICLE)
                    General Review; (REVIEW)
LANGUAGE:           English
FILE SEGMENT:       Priority Journals
ENTRY MONTH:        200308
ENTRY DATE:         Entered STN: 28 Jun 2003
                    Last Updated on STN: 8 Aug 2003
                    Entered Medline: 7 Aug 2003
AB  Poly(ADP-ribose) polymerase-1 (PARP-1) plays a primary role in
    the process of poly(ADP-ribosyl)ation. This posttranslational
    modification of nuclear proteins is activated in response to DNA damage.
    Having been studied for more than 30 years, PARP-1 is now known
    to be implicated in several crucial cellular processes: DNA replication,
    transcription, DNA repair, apoptosis, and genome stability.  In this
    review, we focus on recent findings suggesting that PARP
    -1 participates in DNA damage signaling in cell death.  Of
    clinical relevance is its role in cancer therapy,
    irradiation, and chemotherapy, all of which may cause DNA damage and
    overactivate PARP-1, resulting in inflammation caused by
    necrosis.  Therefore, we will discuss how inhibition of
    PARP-1 may enhance the efficiency of cancer therapy.


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 NEWS  6  NOV 10  CA/CAplus F-Term thesaurus enhanced
 NEWS  7  NOV 10  STN Express with Discover! free maintenance release Version
                  8.01c now available
 NEWS  8  NOV 20  CAS Registry Number crossover limit increased to 300,000 in
                  additional databases
 NEWS  9  NOV 20  CA/CAplus to MARPAT accession number crossover limit increased
                  to 50,000
 NEWS 10  DEC 01  CAS REGISTRY updated with new ambiguity codes
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 NEWS 13  DEC 14  GBFULL and FRFULL enhanced with IPC 8 features and
                  functionality
 NEWS 14  DEC 18  CA/CAplus pre-1967 chemical substance index entries enhanced
                  with preparation role
 NEWS 15  DEC 18  CA/CAplus patent kind codes updated
 NEWS 16  DEC 18  MARPAT to CA/CAplus accession number crossover limit increased
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 NEWS 17  DEC 18  MEDLINE updated in preparation for 2007 reload
 NEWS 18  DEC 27  CA/CAplus enhanced with more pre-1907 records
 NEWS 19  JAN 08  CHEMLIST enhanced with New Zealand Inventory of Chemicals
 NEWS 20  JAN 16  CA/CAplus Company Name Thesaurus enhanced and reloaded
 NEWS 21  JAN 16  IPC version 2007.01 thesaurus available on STN
 NEWS 22  JAN 16  WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
 NEWS 23  JAN 22  CA/CAplus updated with revised CAS roles
 NEWS 24  JAN 22  CA/CAplus enhanced with patent applications from India

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               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
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chain nodes :
19
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  22
chain bonds :
3-19
ring bonds :
1-2  1-6  1-7  2-3  2-10  3-4  4-5  5-6  6-11  7-8  7-22  8-9  9-10  11-12  11-13
12-16  12-22  13-14  14-15  15-16
exact/norm bonds :
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12-22
normalized bonds :
2-10  8-9  9-10  13-14  14-15  15-16
isolated ring systems :
containing 1 :

G1:O,S,N

G2:O,S

G3:C,O,S,N

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  19:CLASS  22:CLASS



L1      STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1              STR
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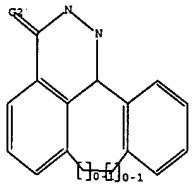

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G1 O,S,N
G2 O,S


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=> S L1 SSS FULL
FULL SEARCH INITIATED 13:37:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      7248 TO ITERATE

100.0% PROCESSED     7248 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L2            0 SEA SSS FUL L1

=> FILE CAPLUS
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                                              ENTRY    SESSION
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                                              ENTRY    SESSION
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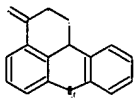

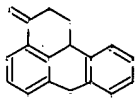

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ring nodes :
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chain bonds :
3-19
ring bonds :
1-2 1-6 1-7 2-3 2-10 3-4 4-5 5-6 6-11 7-8 7-22 8-9 9-10 11-12 11-13
12-16 12-22 13-14 14-15 15-16
exact/norm bonds :
1-2 1-6 1-7 2-3 3-4 3-19 4-5 5-6 6-11 7-8 7-22 11-12 11-13 12-16
12-22
normalized bonds :
2-10 8-9 9-10 13-14 14-15 15-16
isolated ring systems :
containing 1 :

G1:O,S,N

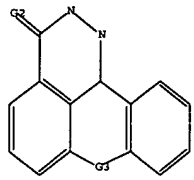
G2:O,S

G3:C,O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 19:CLASS 22:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S,N
G2 O,S
G3 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 15:03:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8 TO 329
PROJECTED ANSWERS: 5 TO 234

L2 5 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 15:03:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 275 TO ITERATE

100.0% PROCESSED 275 ITERATIONS 140 ANSWERS
SEARCH TIME: 00.00.01

L3 140 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 15:03:55 ON 24 JAN 2007
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=> s l3
L4 28 L3

=> d 1-28 ibib abs hitstr

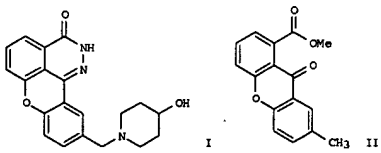
L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:733186 CAPLUS
DOCUMENT NUMBER: 145:188890
TITLE: Preparation of diazabenzoanthracen-3-one compounds as poly(ADP-ribose)polymerase (PARP) inhibitors
INVENTOR(S): Xu, Weizheng; Delahanty, Greg; Zhang, Jie
PATENT ASSIGNEE(S): MGI GP, Inc., USA
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006078711	A2	20060727	WO 2006-US1729	20060119
WO 2006078711	A3	20060921		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-644584P P 20050119
US 2005-712140P P 20050830

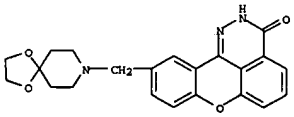
GI



AB About 20 diazabenzoanthracen-3-one compds., such as I, were prepared as poly(ADP-ribose)polymerase (PARP) inhibitors, via (1) bromination of the Me group of II, (2) amination of the resultant bromide with an amine, and (3) cyclocondensation with hydrazine. Their pharmaceutically acceptable salts, hydrates, esters, solvates, and mixts. are claimed. Several biol. activities were tested, I showing PARP inhibition with an IC50 of 0.04 μM. Therefore, the invented compds. and their pharmaceutical compns. are useful for the treatment and/prevention of diseases such as tissue damage and cancer.

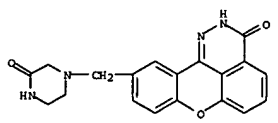
IT 902129-02-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of diazabenzoanthracenone compds. as PARP inhibitors)

RN 902129-02-6 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(1,4-dioxa-8-azaspiro[4.5]dec-8-ylmethyl)-(9CI) (CA INDEX NAME)

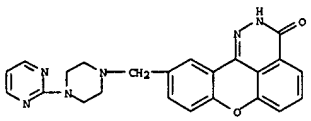


IT 805243-21-4P 805243-22-5P 805243-23-6P
805243-24-7P 902128-84-1P 902128-86-3P
902128-88-5P 902128-90-9P 902128-92-1P
902128-94-3P 902128-96-5P 902128-98-7P
902129-00-4P 902129-04-8P 902129-06-0P
902129-08-2P 902129-10-6P 902129-12-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of diazabenzoanthracenone compds. as PARP inhibitors)

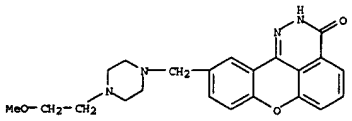
RN 805243-21-4 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(3-oxo-1-piperazinyl)methyl]-(9CI) (CA INDEX NAME)



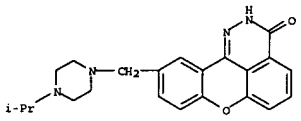
RN 805243-22-5 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(2-pyrimidinyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



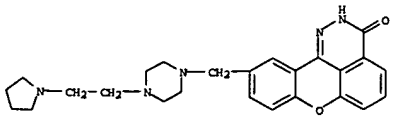
RN 805243-23-6 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(2-methoxyethyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



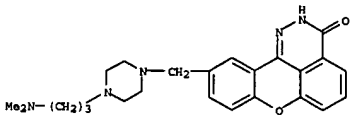
RN 805243-24-7 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(1-methylethyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



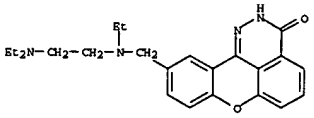
RN 902128-84-1 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-[2-(1-pyrrolidinyl)ethyl]-1-piperazinyl]methyl]-(9CI) (CA INDEX NAME)



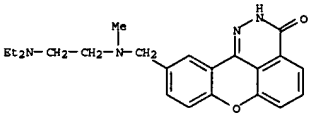
RN 902128-86-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-[3-(dimethylamino)propyl]-1-piperazinyl]methyl]-(9CI) (CA INDEX NAME)



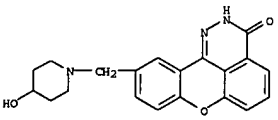
RN 902128-88-5 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[[2-(diethylamino)ethyl]ethylamino]methyl]-(9CI) (CA INDEX NAME)



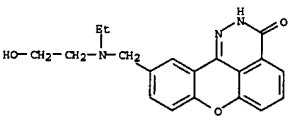
RN 902128-90-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[[2-(diethylamino)ethyl]methylamino]methyl]-(9CI) (CA INDEX NAME)



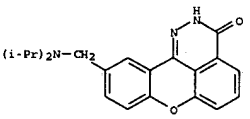
RN 902128-92-1 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(4-hydroxy-1-piperidinyl)methyl]- (9CI) (CA INDEX NAME)



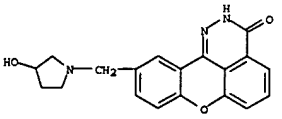
RN 902128-94-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[ethyl(2-hydroxyethyl)amino]methyl]- (9CI) (CA INDEX NAME)



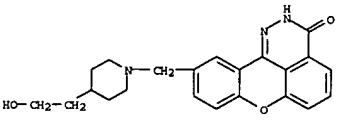
RN 902128-96-5 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[bis(1-methylethyl)amino]methyl]- (9CI) (CA INDEX NAME)



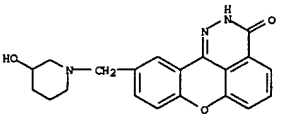
RN 902128-98-7 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(3-hydroxy-1-pyrrolidinyl)methyl]- (9CI) (CA INDEX NAME)



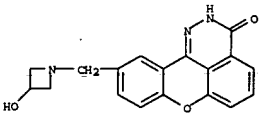
RN 902129-00-4 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(2-hydroxyethyl)-1-piperidinyl]methyl]- (9CI) (CA INDEX NAME)



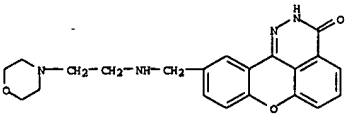
RN 902129-04-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(3-hydroxy-1-piperidinyl)methyl]- (9CI) (CA INDEX NAME)



RN 902129-06-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(3-hydroxy-1-azetidinyl)methyl]- (9CI) (CA INDEX NAME)

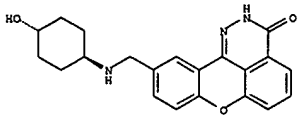


RN 902129-08-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[[2-(4-morpholinyl)ethyl]amino]methyl]- (9CI) (CA INDEX NAME)

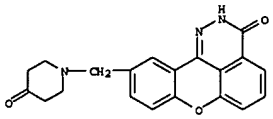


RN 902129-10-6 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[(trans-4-hydroxycyclohexyl)amino]methyl]- (9CI) (CA INDEX NAME)

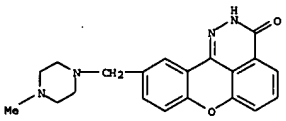
Relative stereochemistry.



RN 902129-12-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(4-oxo-1-piperidinyl]methyl]- (9CI) (CA INDEX NAME)

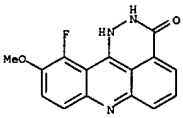


L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1276816 CAPLUS
DOCUMENT NUMBER: 144:121270
TITLE: Treatment with PARP-1 inhibitors, GPI 15427 or GPI 16539, ameliorates intestinal damage in rat models of colitis and shock
AUTHOR(S): Di Paola, Rosanna; Mazzon, Emanuela; Xu, Weizheng; Genovese, Tiziana; Ferrraris, Dana; Muia, Carmelo; Crisafulli, Concetta; Zhang, Jie; Cuzzocrea, Salvatore
CORPORATE SOURCE: Department of Clinical and Experimental Medicine and Pharmacology, Torre Biologica, School of Medicine, Torre Biologica, University of Messina, Policlinico Universitario Via C. Valeria, Messina, 98100, Italy
SOURCE: European Journal of Pharmacology (2005), 527(1-3), 163-171
CODEN: EJPHAZ; ISSN: 0014-2999
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Poly (ADP-ribose) polymerase-1 (PARP-1), a nuclear enzyme activated by DNA strand breaks, plays a detrimental role during inflammation. As inflammation is important in the development of colitis and ischemia/reperfusion (I/R) injury of the intestine, we investigated the effects of 10-(4-methyl-piperazin-1-ylmethyl)-2H-7-oxa-1,2-diaza-benzo[de]anthracen-3-one (GPI 15427) and 2-(4-methyl-piperazin-1-yl)-5H-benzo[c][1,5]naphthyridin-6-one (GPI 16539), two novel and potent inhibitors of PARP-1, in a rat model of gut injury and inflammation, splanchnic artery occlusion (SAO) shock and dinitrobenzene sulfonic acid (DNBS)-induced colitis. We report here for the first time that post-injury administration of GPI 15427 and GPI 16539 exerts potent anti-inflammatory effects by reducing inflammatory cell infiltration and histol. injury, and delaying the development of clin. signs in both in vivo models. Furthermore, GPI 15427 and GPI 16539 treatment diminished the accumulation of poly(ADP-ribose) in the ileum of splanchnic artery occlusion-shocked rats and in the colons of dinitrobenzene sulfonic acid-treated rats. Thus, GPI 15427 and GPI 16539 exhibited anti-inflammation activity against damage caused by intestinal ischemia/reperfusion and colitis. GPI 15427 and GPI 16539 may be useful for treating gut ischemia and inflammation.
IT 805242-85-7
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(PARP-1 inhibitors GPI 15427 or GPI 16539 ameliorate intestinal damage in colitis and shock)
RN 805242-85-7 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(4-methyl-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



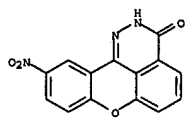
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:485716 CAPLUS
DOCUMENT NUMBER: 143:172738
TITLE: A Convenient Route to Diverse Heterocycles through an Addition of β-Amino Carbonyl Compounds to 3-Halogeno-4-methoxybenzynes
AUTHOR(S): Yoon, Kyongho; Ha, Sung Min; Kim, Kyongtae
CORPORATE SOURCE: School of Chemistry and Molecular Engineering, Seoul National University, Seoul, 151-742, S. Korea
SOURCE: Journal of Organic Chemistry (2005), 70(14), 5741-5744
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 3-Halo-4-methoxybenzyne deriva. generated from 5-(3-halo-4-methoxyphenyl)thianthreniumperchlorate deriva. 1 and LDA in THF at reflux reacted with various β-amino carbonyl compds. and 2-aminophenyl benzenesulfonate etc. to give diverse heterocyclic compds. For example, the addition reaction of fluoro methoxy benzyne derived from 5-(3-fluoro-4-methoxyphenyl)thianthreniumperchlorate to 2-amino-benzophenone gave 1-fluoro-2-methoxy-9-phenyl-acridine.
IT 861149-78-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of heterocyclic compds. via addition of β-amino carbonyl compds. to (halo)(methoxy)benzyne deriva.)
RN 861149-78-2 CAPLUS
CN 3H-Pyridazino[5,4,3-kl]acridin-3-one,11-fluoro-1,2-dihydro-10-methoxy- (9CI) (CA INDEX NAME)



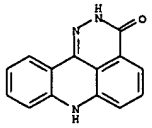
REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:331743 CAPLUS
DOCUMENT NUMBER: 143:37901
TITLE: Including Tightly-Bound Water Molecules in de Novo Drug Design. Exemplification through the in Silico Generation of Poly(ADP-ribose)polymerase Ligands
AUTHOR(S): Garcia-Sosa, Alfonso T.; Firth-Clark, Stuart; Mancera, Ricardo L.
CORPORATE SOURCE: Department of Pharmacology, University of Cambridge, Cambridge, CB2 1PD, UK
SOURCE: Journal of Chemical Information and Modeling (2005), 45(3), 624-633
CODEN: JCISD8; ISSN: 1549-9596
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Different strategies for the in silico generation of ligand mols. in the binding site of poly(ADP-ribose)polymerase (PARP) were studied in order to observe the effect of the targeting and displacement of tightly bound water mols. Several mol. scaffolds were identified as having better interactions in the binding site when targeting one or two tightly bound water mols. in the NAD binding site. Energy calcns. were conducted in order to assess the ligand-protein and ligand-water-protein interactions of different functional groups of the generated ligands. These calcns. were used to evaluate the energetic consequences of the presence of tightly bound water mols. and to identify those that contribute favorably to the binding of ligands.
IT 220938-25-0, WD 99-004345
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(including tightly-bound water mols. in de novo drug design and exemplification through the in silico generation of poly(ADP-ribose)polymerase ligands)
RN 220938-25-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-nitro- (9CI) (CA INDEX NAME)

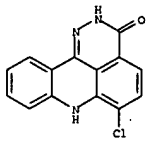


REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:150030 CAPLUS
DOCUMENT NUMBER: 142:366757
TITLE: 2,7-Dihydro-3H-pyridazino[5,4,3-kl]acridin-3-one derivatives, novel type of cytotoxic agents active on multidrug-resistant cell lines. Synthesis and biological evaluation
AUTHOR(S): Stefanska, Barbara; Bontemps-Gracz, Maria M.; Antonini, Ippolito; Martelli, Sante; Arciemiuk, Malgorzata; Piwkowska, Agnieszka; Rogacka, Dorota; Borowski, Edward
CORPORATE SOURCE: Department of Pharmaceutical Technology and Biochemistry, Gdansk University of Technology, Gdansk, 80-952, Pol.
SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(6), 1969-1975
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:366757
AB We have earlier postulated that the presence of a pyridazone ring fused with an anthracenedione moiety resulted in the analog's ability to overcome multidrug resistance of tumor cells (J. Med. Chemical 1999, 42, 3494). High cytotoxic activity of obtained anthrapyridazones (Bioorg. Med. Chemical 2003, 11, 561) toward the resistant cell lines, prompted us to synthesize the similarly modified acridine compds. A series of pyridazinoacridin-3-one deriv. (2b-h) were prepared from the reaction of 9-oxo-9,10-dihydroacridine-1-carboxylatewith POCl3, followed by addition of the appropriate (alkylamino)alkylhydrazines. In vitro cytotoxic activity toward sensitive and resistant leukemia cell lines: L1210, K562, K562/DX, HL-60, HL-60/VINC, and HL-60/DX, with various type of multidrug resistance (MDR and MRP) was determined. The compds. studied exhibited in comparison to the reference cytostatics (DX, MIT) desirable very low resistance indexes (RI). Variations have been observed depending upon the substituent and the type of drug exporting pump. The cytotoxic activities of examined compds., as well as of model anthrapyridazone derivative PDZ, were lower than those of reference drugs (DX, MIT) due to their diminished affinity to DNA.
IT 849405-26-1P 849405-33-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and structure-activity relationship studies of 2,7-Dihydro-3H-pyridazino[5,4,3-kl]acridin-3-onederivs., as novel cytotoxic agents in multidrug-resistant leukemia cell lines)
RN 849405-26-1 CAPLUS
CN 3H-Pyridazino[5,4,3-kl]acridin-3-one,2,7-dihydro- (9CI) (CA INDEX NAME)



RN 849405-33-0 CAPLUS
CN 3H-Pyridazino[5,4,3-kl]acridin-3-one,6-chloro-2,7-dihydro- (9CI) (CA INDEX NAME)



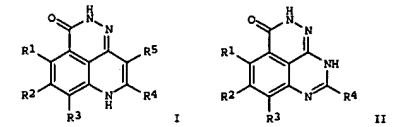
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1059130 CAPLUS
DOCUMENT NUMBER: 142:38268
TITLE: Preparation of fused tricyclic nitrogen compounds as poly(ADP-ribose) polymerase inhibitors
INVENTOR(S): Kalish, Vincent J.; Zhang, Jie; Xu, Weizheng; Li, Jia-He; Xing, Amy D.
PATENT ASSIGNEE(S): Guildford Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

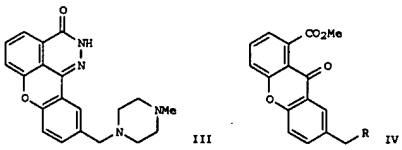
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004105700	A2	20041209	WO 2004-US16524	20040526
WO 2004105700	A3	20050414		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004242947	A1	20041209	AU 2004-242947	20040526
CA 2527420	A1	20041209	CA 2004-2527420	20040526
US 2005020595	A1	20050127	US 2004-853714	20040526
EP 1633362	A2	20060315	EP 2004-753367	20040526
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				

PRIORITY APPLN. INFO.: US 2003-473475P P 20030528
WO 2004-US16524 W 20040526

OTHER SOURCE(S): MARPAT 142:38268
GI



I II

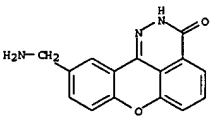


III IV

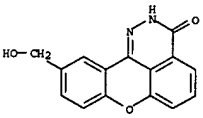
AB The present invention provides fused tricyclic nitrogen heterocycles I and II [R1, R2 = independently H, halo, alkoxy, lower alkyl; R3-R5 = independently H, OH, carboxy, (un)substituted amino, hydrazino, alkoxy, aryloxy, alkyl, alkenyl, alkynyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl, etc.] as compds. which inhibit poly(ADP-ribose) polymerase (PARP), compns. containing these compds. and methods for using these PARP inhibitors to treat, prevent and/or ameliorate the effects of the conditions described herein. Also described are benzopyrano[4,3,2-de]phthalazinones, e.g. III. Thus, bromination of oxoxanthene ester IV (R = H) with NBS in CCl4 gave 45% bromide IV (R = Br), which underwent substitution with N-methylpiperazine to give 59% IV (R = 4-methyl-1-piperazino). Cyclocondensation of IV (R = 4-methyl-1-piperazino) with N2H4 gave III in 98% yield. III was tested for focal cerebral ischemia effect, myocardial protection, and sensitization of human cancer cell lines to temozolomide (TMZ)treatment.

IT 805242-91-5P 805242-99-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of fused tricyclic nitrogen compds. as poly(ADP-ribose) polymerase inhibitors)

RN 805242-91-5 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(aminomethyl)- (9CI) (CA INDEX NAME)

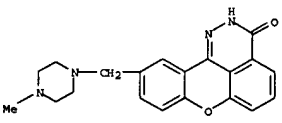


RN 805242-99-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(hydroxymethyl)- (9CI) (CA INDEX NAME)

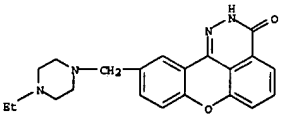


IT 805242-85-7P 805242-86-8P 805242-87-9P
805242-88-0P 805242-89-1P 805242-90-4P
805242-93-7P 805242-94-8P 805242-95-9P
805242-96-0P 805242-97-1P 805242-98-2P
805243-00-9P 805243-01-0P 805243-02-1P
805243-03-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fused tricyclic nitrogen compds. as poly(ADP-ribose) polymerase inhibitors)

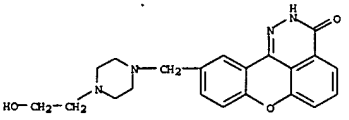
RN 805242-85-7 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(4-methyl-1-piperazinyl)methyl]- (9CI) (CA INDEX NAME)



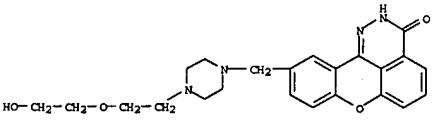
RN 805242-86-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(4-ethyl-1-piperazinyl)methyl]- (9CI) (CA INDEX NAME)



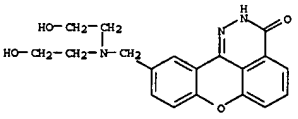
RN 805242-87-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(2-hydroxyethyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



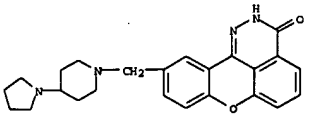
RN 805242-88-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-[(2-hydroxyethoxy)ethyl]-1-piperazinyl]methyl]-(9CI) (CA INDEX NAME)



RN 805242-89-1 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[bis(2-hydroxyethyl)amino]methyl]- (9CI) (CA INDEX NAME)

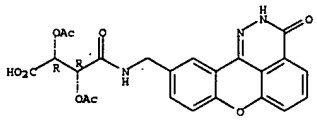


RN 805242-90-4 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(1-pyrrolidinyl)-1-piperidinyl]methyl]- (9CI) (CA INDEX NAME)



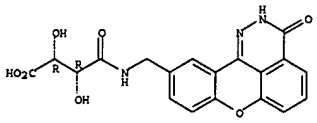
RN 805242-93-7 CAPLUS
CN Butanoic acid, 2,3-bis(acetyloxy)-4-[[[2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl]amino]-4-oxo-(2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



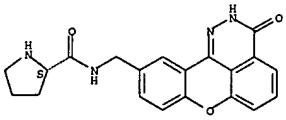
RN 805242-94-8 CAPLUS
CN Butanoic acid, 4-[[(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl]amino]-2,3-dihydroxy-4-oxo-,(2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

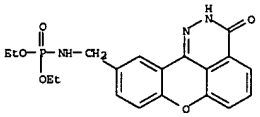


RN 805242-95-9 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-[(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl]-, (2S)- (9CI) (CA INDEX NAME)

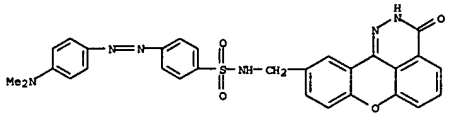
Absolute stereochemistry.



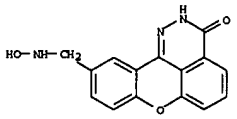
RN 805242-96-0 CAPLUS
CN Phosphoramidic acid, [(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl]-, diethyl ester (9CI) (CA INDEX NAME)



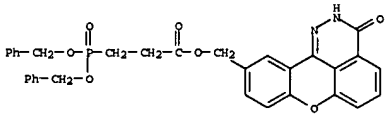
RN 805242-97-1 CAPLUS
CN Benzenesulfonamide, N-[(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl]-4-[[4-(dimethylamino)phenyl]azo]-(9CI) (CA INDEX NAME)



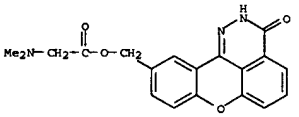
RN 805242-98-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(hydroxyamino)methyl]-(9CI) (CA INDEX NAME)



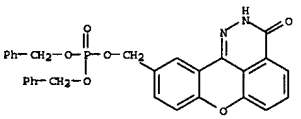
RN 805243-00-9 CAPLUS
CN Propanoic acid, 3-[bis(phenylmethoxy)phosphinyl]-, (2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methylester (9CI) (CA INDEX NAME)



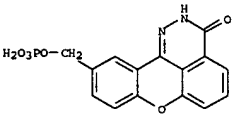
RN 805243-01-0 CAPLUS
CN Glycine, N,N-dimethyl-, (2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl ester (9CI) (CA INDEX NAME)



RN 805243-02-1 CAPLUS
CN Phosphoric acid, (2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

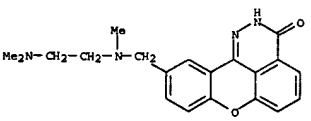


RN 805243-03-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(phosphonooxy)methyl]-(9CI) (CA INDEX NAME)

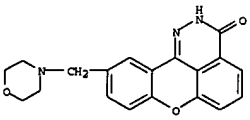


IT 328526-29-0 328526-31-4 805243-17-8
805243-18-9 805243-19-0 805243-20-3
805243-21-4 805243-22-5 805243-23-6
805243-24-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of fused tricyclic nitrogen compds. as poly(ADP-ribose) polymerase inhibitors)

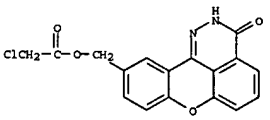
RN 328526-29-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[[2-(dimethylamino)ethyl]methylamino]methyl]-(9CI) (CA INDEX NAME)



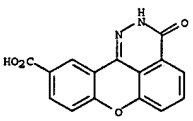
RN 328526-31-4 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(4-morpholinylmethyl)-(9CI) (CA INDEX NAME)



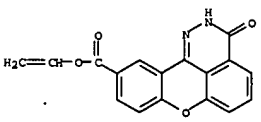
RN 805243-17-8 CAPLUS
CN Acetic acid, chloro-, (2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl ester (9CI) (CA INDEX NAME)



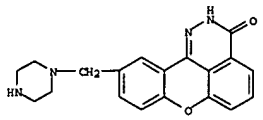
RN 805243-18-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-carboxylicacid, 2,3-dihydro-3-oxo-(9CI) (CA INDEX NAME)



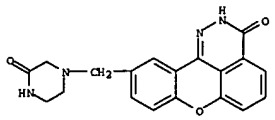
RN 805243-19-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-carboxylicacid, 2,3-dihydro-3-oxo-, ethenyl ester (9CI) (CA INDEX NAME)



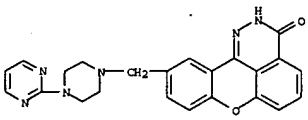
RN 805243-20-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(1-piperazinylmethyl)-(9CI) (CA INDEX NAME)



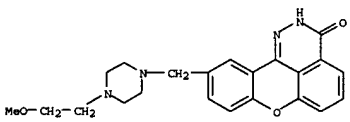
RN 805243-21-4 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(3-oxo-1-piperazinyl)methyl]- (9CI) (CA INDEX NAME)



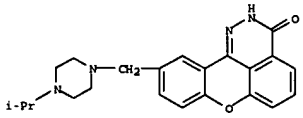
RN 805243-22-5 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(2-pyrimidinyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



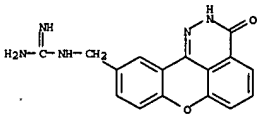
RN 805243-23-6 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(2-methoxyethyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



RN 805243-24-7 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(1-methylethyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)

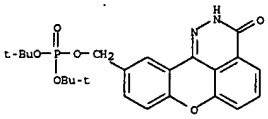


IT 805242-92-6P 805243-05-4P 805243-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fused tricyclic nitrogen compds. as poly(ADP-ribose) polymerase inhibitors)
RN 805242-92-6 CAPLUS
CN Guanidine, [(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



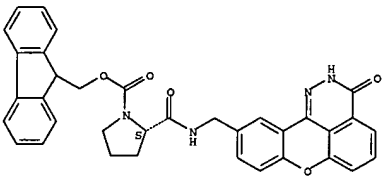
● HCl

RN 805243-05-4 CAPLUS
CN Phosphoric acid, (2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 805243-11-2 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, 2-[[[(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl]amino]carbonyl]-,9H-fluoren-9-ylmethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

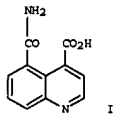


L4 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:829353 CAPLUS
DOCUMENT NUMBER: 139:317471
TITLE: Aryl and heteroaryl poly(ADP-ribose) polymerase (PARP) inhibitors, preparation, pharmaceutical compositions, and methods of therapeutic use
INVENTOR(S): Jackson, Paul F.; Li, Jia-He; Maclin, Keith M.; Zhang, Jie
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: U.S., 37 pp., Cont.-in-part of U.S. Ser. No. 79,512, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6635642	B1	20031021	US 1998-145176	19980901
US 6346536	B1	20020212	US 1997-922548	19970903
CA 2294074	A1	19990311	CA 1998-2294074	19980902
WO 9911649	A2	19990311	WO 1998-US18185	19980902
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9893748	A	19990322	AU 1998-93748	19980902
EP 1012153	A1	20000628	EP 1998-946812	19980902
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

PRIORITY APPLN. INFO.: US 1997-922520 B2 19970903
US 1997-922548 A2 19970903
US 1998-79512 B2 19980515
US 1998-145176 A 19980901
WO 1998-US18185 W 19980902

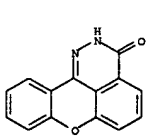
GI



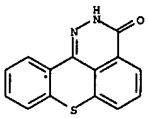
I

AB The invention discloses PARP inhibitors, pharmaceutical compns. comprising them, and methods of using them to treat tissue damage resulting from cell damage or death due to necrosis or apoptosis, effect neuronal activities not mediated by NMDA toxicity; to treat neural tissue damage resulting from ischemia and reperfusion injury, neurol. disorders and neurodegenerative diseases; to prevent or treat vascular stroke; to treat or prevent cardiovascular disorders; to treat other conditions and/or disorders such as age-related macular degeneration, AIDS and other immune senescence diseases, arthritis, atherosclerosis, cachexia, cancer, degenerative diseases of skeletal muscle involving replicative senescence, diabetes, head trauma, immune senescence, inflammatory bowel disorders (such as colitis and Crohn's disease), muscular dystrophy, osteoarthritis, osteoporosis, chronic and/or acute pain (such as neuropathic pain), renal failure, retinal ischemia, septic shock (such as endotoxic shock), organ damage due to transplantation, and skin aging; to extend the lifespan and proliferative capacity of cells; to alter gene expression of senescent cells; or to radiosensitize hypoxic tumor cells. Preparation of e.g. carboxamide PARP inhibitor I is described. The neuroprotective effect of 3,4-dihydro-5-[4-(1-piperidinyl)butoxy]-1(2H)-isoquinolinonis presented. Effects of compds. of the invention on e.g. heart ischemia/reperfusion injury are also described.

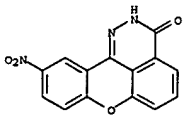
IT 220938-23-8 220938-24-9 220938-25-0
220938-26-1
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(aryl and heteroaryl PARP inhibitors, preparation, pharmaceutical compns., and therapeutic use)
RN 220938-23-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one(9CI) (CA INDEX NAME)



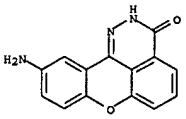
RN 220938-24-9 CAPLUS
CN [1]Benzothiopyrano[4,3,2-de]phthalazin-3(2H)-one(9CI) (CA INDEX NAME)



RN 220938-25-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-nitro- (9CI) (CA INDEX NAME)



RN 220938-26-1 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-amino- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 528 THERE ARE 528 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

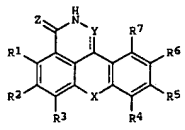
L4 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:92405 CAPLUS
DOCUMENT NUMBER: 138:137290
TITLE: Preparation of benzpyranoisoquinolinones and related compounds as poly(ADP-ribose)polymerase (PARP) inhibitors.
INVENTOR(S): Li, Jia-He; Zhang, Jie; Jackson, Paul F.; Maclin, Keith M.
PATENT ASSIGNEE(S): Guilford Pharmaceuticals, Inc., USA
SOURCE: U.S., 41 pp., Cont.-in-part of U.S. 6,306,889.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6514983	B1	20030204	US 1998-145181	19980901
US 6346536	B1	20020212	US 1997-922548	19970903
US 6306889	B1	20011023	US 1998-47502	19980325
CA 2294133	A1	19990311	CA 1998-2294133	19980902
WO 9911645	A1	19990311	WO 1998-US18189	19980902
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9892982	A	19990322	AU 1998-92982	19980902
BR 9812185	A	20000718	BR 1998-12185	19980902
EP 1019409	A1	20000719	EP 1998-945828	19980902
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
TR 200001279	T2	20001023	TR 2000-200001279	19980902
HU 200003569	A2	20010730	HU 2000-3569	19980902
JP 2002510332	T	20020402	JP 1999-516974	19980902
NZ 503043	A	20021025	NZ 1998-503043	19980902
NO 2000001001	A	20000405	NO 2000-1001	20000228

PRIORITY APPLN. INFO.:

US 1997-922548	A2	19970903
US 1998-47502	A2	19980325
US 1998-145181	A	19980901
WO 1998-US18189	W	19980902

OTHER SOURCE(S): MARPAT 138:137290
GI

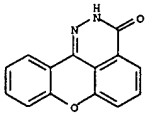


I

AB Title compds. [I; Y = alkylhalo, alkyl-COG, COG, bond, CO, O, NR11, CR8; G = NR11 R16, OR9, SR9, R10 ; Z = O, S, NR11; X = NR16, O, S, CR12R13, CO, bond, CR12:CR13, CR12 R13CR14R15; R1-R8, R10, R12-R15 = H, halo, alkylhalo, OH, alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, amino, alkylamino, NO2, nitroso, CO2H, aralkyl; R9 = H, OH, alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, amino, alkylamino, CO2H, aralkyl; R11, R16 = H, halo, alkylhalo, OH, alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, amino, alkylamino, CO2H, aralkyl; the alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, aralkyl groups may be substituted; with provisos], were prepared Thus, 9-xanthenylmethyl isocyanate (preparation given) was heated in polyphosphoric acid at 90° to give 1,11b-dihydrobenzopyrano[4,3,2-de]isoquinolin-3-one. The latter inhibited PARP with IC50 = 0.20 μM.

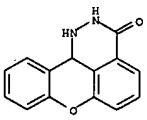
IT 220938-23-8
RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(preparation of benzpyranoisoquinolinones and related compds. as PARP inhibitors)

RN 220938-23-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one(9CI) (CA INDEX NAME)



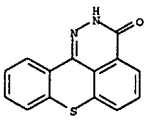
IT 220938-19-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzpyranoisoquinolinones and related compds. as PARP inhibitors)

RN 220938-19-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,1,11b-dihydro- (9CI) (CA INDEX NAME)

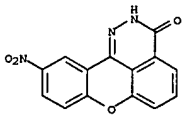


IT 220938-24-9 220938-25-0 220938-26-1
220938-28-3 220938-32-9 220938-35-2
220938-36-3 220938-37-4 220938-39-6
220938-40-9 220938-42-1
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of benzpyranoisoquinolinones and related compds. as PARP inhibitors)

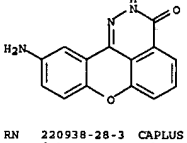
RN 220938-24-9 CAPLUS
CN [1]Benzothiopyrano[4,3,2-de]phthalazin-3(2H)-one(9CI) (CA INDEX NAME)



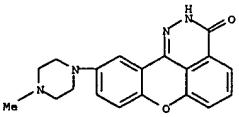
RN 220938-25-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-nitro- (9CI) (CA INDEX NAME)



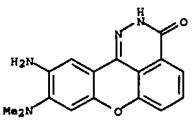
RN 220938-26-1 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-amino- (9CI) (CA INDEX NAME)



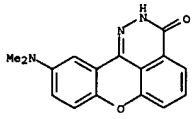
RN 220938-28-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



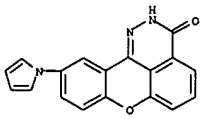
RN 220938-32-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-amino-9-(dimethylamino)- (9CI) (CA INDEX NAME)



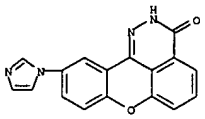
RN 220938-35-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(dimethylamino)- (9CI) (CA INDEX NAME)



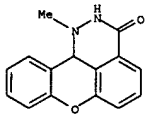
RN 220938-36-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(1H-pyrrol-1-yl)- (9CI) (CA INDEX NAME)



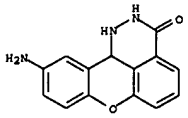
RN 220938-37-4 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(1H-imidazol-1-yl)- (9CI) (CA INDEX NAME)



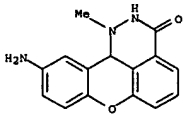
RN 220938-39-6 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,1,11b-dihydro-1-methyl- (9CI) (CA INDEX NAME)



RN 220938-40-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-amino-1,11b-dihydro- (9CI) (CA INDEX NAME)

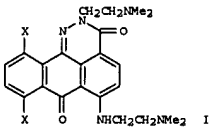


RN 220938-42-1 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-amino-1,11b-dihydro-1-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 567 THERE ARE 567 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:52765 CAPLUS
DOCUMENT NUMBER: 140:16693
TITLE: Synthesis and biological evaluation of 2,7-dihydro-3H-dibenzo[de,h]cinnoline-3,7-dione derivatives, a novel group of anticancer agents active on a multidrug resistant cell line
AUTHOR(S): Stefanska, Barbara; Arciemiuk, Malgorzata; Bontemps-Gracz, Maria M.; Dzieduszycka, Maria; Kupiec, Agnieszka; Martelli, Sante; Borowski, Edward
CORPORATE SOURCE: Department of Pharmaceutical Technology and Biochemistry, Gdansk University of Technology, Gdansk,. 80-952, Pol.
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(4), 561-572
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:16693
GI



I

AB Anthrapyridazone derivs. with one or two basic side chains at various positions in the tetracyclic chromophore have been synthesized. The key intermediates in the synthesis are 2,7-dihydro-3H-dibenzo[de,h]cinnoline-3,7-diones monosubstituted at position 2 or 6 or disubstituted at positions 2 and 6 or 2 and 8 with appropriate (alkylamino)alkylamines. All analogs showed in vitro cytotoxic activity against murine leukemia (L1210) and human leukemia (K562) cell lines. The compds. were also active against human leukemia multidrug resistant (K562/DX) cell line with resistance index (RI) in the range 1-3 depending on the compound structure. Two of the most active in vitro compds. (I; X = H, OH) were tested in vivo against murine P388 leukemia and displayed antileukemic activity comparable with that of Mitoxantrone. DNA-binding assays were performed and DNA affinity data were correlated with the structures of the compds. The cytoplasmic membrane affinity values (log k'IAM) have also been determined and the correlation with the resistance indexes discussed. The anthrapyridazones constitute a novel group of antitumor compds. that can overcome multidrug resistance.

IT 630128-91-5P 630128-92-6P 630128-93-7P
630128-94-8P 630128-95-9P 630128-96-0P
630129-02-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(2,7-dihydro-3H-dibenzo[de,h]cinnoline-3,7-dionesas antileukemic agents active on multidrug resistant cell line)

RN 630128-91-5 CAPLUS
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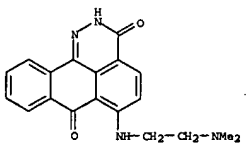
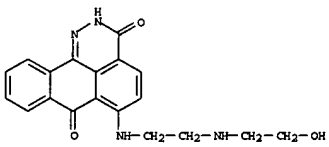


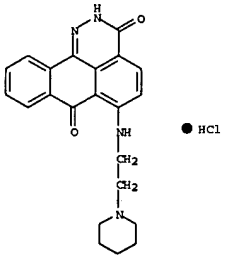
● HCl

RN 630128-92-6 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-[(2-hydroxyethyl)amino]ethyl]amino]-,monohydrochloride (9CI) (CA INDEX NAME)



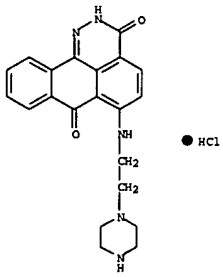
● HCl

RN 630128-93-7 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(1-piperidinyl)ethyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

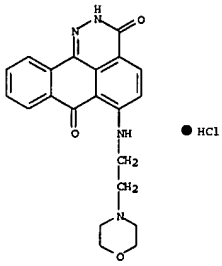


● HCl

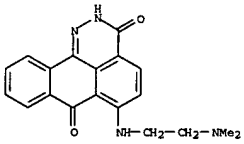
RN 630128-94-8 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(1-piperazinyl)ethyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



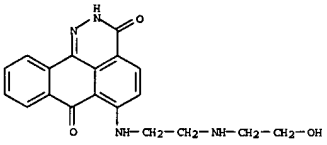
RN 630128-95-9 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(4-morpholinyl)ethyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



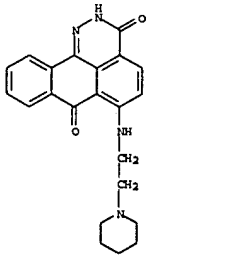
RN 630128-96-0 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(dimethylamino)ethyl]methylamino]-,monohydrochloride (9CI) (CA INDEX NAME)



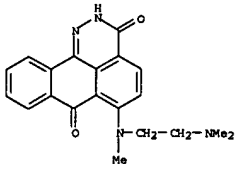
RN 630128-70-0 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-((2-hydroxyethyl)amino]ethyl]amino]-(9CI) (CA INDEX NAME)



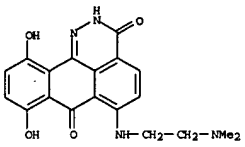
RN 630128-71-1 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(1-piperidinyl)ethyl]amino]-(9CI) (CA INDEX NAME)



RN 630128-72-2 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(1-piperazinyl)ethyl]amino]-(9CI) (CA INDEX NAME)

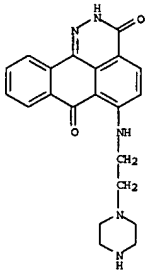


RN 630129-02-1 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(dimethylamino)ethyl]amino]-8,11-dihydroxy-, monohydrochloride (9CI) (CA INDEX NAME)

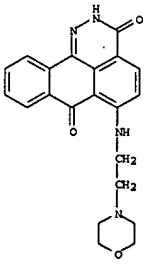


IT 630128-69-7P 630128-70-0P 630128-71-1P
630128-72-2P 630128-73-3P 630128-74-4P
630128-80-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(2,7-dihydro-3H-dibenzo[de,h]cinnoline-3,7-diones as antileukemic agents active on multidrug resistant cell line)

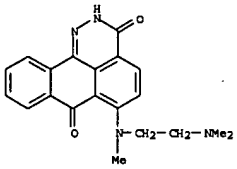
RN 630128-69-7 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(dimethylamino)ethyl]amino]-(9CI) (CA INDEX NAME)



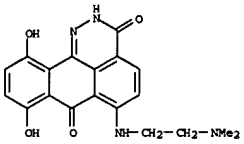
RN 630128-73-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(4-morpholinyl)ethyl]amino]-(9CI) (CA INDEX NAME)



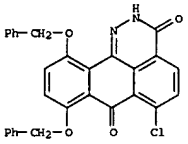
RN 630128-74-4 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(dimethylamino)ethyl]methylamino]-(9CI) (CA INDEX NAME)



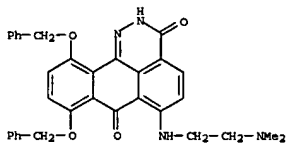
RN 630128-80-2 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(dimethylamino)ethyl]amino]-8,11-dihydroxy- (9CI) (CA INDEX NAME)



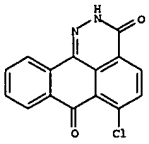
IT 630129-42-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate, amination of; 2,7-dihydro-3H-dibenzo[de,h]cinnoline-3,7-diones as antileukemic agents active on multidrug resistant cell line)
RN 630129-42-9 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-chloro-8,11-bis(phenylmethoxy)- (9CI) (CA INDEX NAME)



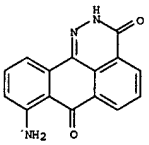
IT 630129-43-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate, deprotection of; 2,7-dihydro-3H-dibenzo[de,h]cinnoline-3,7-diones as antileukemic agents active on multidrug resistant cell line)
RN 630129-43-0 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-[[2-(dimethylamino)ethyl]amino]-8,11-bis(phenylmethoxy)- (9CI) (CA INDEX NAME)



IT 361986-37-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(prereactant, amination of; 2,7-dihydro-3H-dibenzo[de,h]cinnoline-3,7-diones as antileukemic agents active on multidrug resistant cell line)
RN 361986-37-0 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-chloro- (9CI) (CA INDEX NAME)



IT 57981-26-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(prereactant, aminoalkylation of; 2,7-dihydro-3H-dibenzo[de,h]cinnoline-3,7-diones as antileukemic agents active on multidrug resistant cell line)
RN 57981-26-7 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-amino- (7CI, 9CI) (CA INDEX NAME)



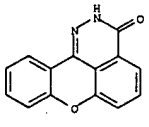
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:815784 CAPLUS
DOCUMENT NUMBER: 138:182963

TITLE: Characterization of competitive inhibitors for the transferase activity of Pseudomonas aeruginosa exotoxin A
AUTHOR(S): Armstrong, Souzan; Li, Jia-He; Zhang, Jie; Merrill, A. Rod
CORPORATE SOURCE: Guelph-Waterloo Centre for Graduate Work in Chemistry and Biochemistry, Department of Chemistry and Biochemistry, University of Guelph, Guelph, ON, N1G 2W1, Can.
SOURCE: Journal of Enzyme Inhibition and Medicinal Chemistry (2002), 17(4), 235-246
CODEN: JEIMAZ; ISSN: 1475-6366
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of small, nonpolar compds. were tested for their ability to inhibit the ADP-ribosyl transferase activity of Pseudomonas aeruginosa exotoxin A. The IC50 values for the compds. tested ranged from 87 nM to 484 μM for NAP and CMP12, resp. It was demonstrated that NAP was a competitive inhibitor of the ADPRT reaction for the NAD+ substrate with a Ki of 45 ± 5 nM, which was in good agreement with the dissociation constant determined independently (KD = 56 ± 6 nM). The IC50 value for NAP was 87 ± 12 nM, which strongly correlated with the Ki and KD values. Furthermore, NAP was shown to noncovalently associate with the exotoxin A active site using exhaustive dialysis, NMR, and electrospray mass spectrometry. Finally, a computer mol. model using the X-ray structure of the substrate-bound toxin was generated with NAP bound to the active site of exotoxin A at the nicotinamide-binding site. This model is consistent with the X-ray structure of the catalytic domain of poly-ADP-ribose polymerase complexed with 4-amino-naphthalimide (Compound 4) that was included in this study.

IT 220938-23-8
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(characterization of naphthalimide and related compds. as competitive inhibitors for ADP-ribosyl transferase activity of Pseudomonas aeruginosa exotoxin A)
RN 220938-23-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one(9CI) (CA INDEX NAME)



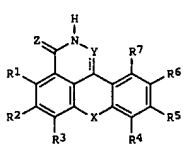
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:772134 CAPLUS
DOCUMENT NUMBER: 135:318418
TITLE: Preparation of [1]1,10b-dihydrobenzopyrano[4,3,2-de]isoindolin-1-one and its analogs as novel poly(ADP-ribose) polymerase (PARP) inhibitors
INVENTOR(S): Li, Jia-He; Zhang, Jie; Jackson, Paul F.; Maclin, Keith M.
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: U.S., 24 pp., Cont.-in-part of U.S. Ser. No. 922,548.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6306889	B1	20011023	US 1998-47502	19980325
US 6346536	B1	20020212	US 1997-922548	19970903
US 6514983	B1	20030204	US 1998-145181	19980901
ZA 9808016	A	19990303	ZA 1998-8016	19980902
ZA 9808017	A	19990303	ZA 1998-8017	19980902
CA 2294133	A1	19990311	CA 1998-2294133	19980902
WO 9911645	A1	19990311	WO 1998-US18189	19980902
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9892982	A	19990322	AU 1998-92982	19980902
BR 9812185	A	20000718	BR 1998-12185	19980902
EP 1019409	A1	20000719	EP 1998-945828	19980902
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
TR 200001279	T2	20001023	TR 2000-200001279	19980902
HU 200003569	A2	20010730	HU 2000-3569	19980902
JP 2002510332	T	20020402	JP 1999-516974	19980902
NZ 503043	A	20021025	NZ 1998-503043	19980902
NO 2000001001	A	20000405	NO 2000-1001	20000228

PRIORITY APPLN. INFO.:
US 1997-922548 A2 19970903
US 1998-47502 A2 19980325
US 1998-145181 A 19980901
WO 1998-US18189 W 19980902

OTHER SOURCE(S): MARPAT 135:318418
GI



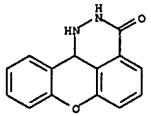
I

AB The title compds. [I; Y = alkylhalo, a direct bond, CO, etc.; Z = O, S, NR11; X = NR12, O, S, etc.; R1-R7, R11, R12 = H, halo, alkyl, etc.], useful for the treatment or prevention of neural or cardiovascular tissue damage related to cerebral ischemia and reperfusion injury in an animal, were prepared Thus, hydrogenating a mixture of Me 9-oxoxanthene-1-carboxylate (preparation given) with NH4OAc and glacial AcOH over 10% Pd/C in a bomb at 2000 psi afforded 30% I [Y = a direct bond; X = O; Z = O; R1-R7 = H]. The compds. I showed IC50's in range of a few nM to 20 μM in PARP assay.

IT 220938-19-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of [1]1,10b-dihydrobenzopyrano[4,3,2-de]isoindolin-1-onand its analogs as novel poly(ADP-ribose) polymerase (PARP) inhibitors)

RN 220938-19-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,1,11b-dihydro- (9CI) (CA INDEX NAME)



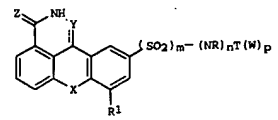
REFERENCE COUNT: 345 THERE ARE 345 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:167996 CAPLUS
DOCUMENT NUMBER: 134:207821
TITLE: Preparation of [1]benzopyrano[4,3,2-de]phthalazine-3(2H)-ones, pharmaceutical compositions and use for treating cellular damage, such as neural or cardiovascular tissue damage
INVENTOR(S): Li, Jia-He; Zhang, Jie
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

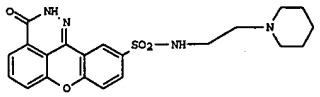
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001016137	A1	20010308	WO 2000-US23745	20000830
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6291425	B1	20010918	US 1999-387767	19990901
CA 2382317	A1	20010308	CA 2000-2382317	20000830
EP 1212328	A1	20020612	EP 2000-959578	20000830
EP 1212328	B1	20060802		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003508400	T	20030304	JP 2001-519703	20000830
AT 334985	T	20060815	AT 2000-959578	20000830
US 6716828	B1	20040406	US 2001-781195	20010213
US 2005074470	A1	20050407	US 2004-772235	20040206
AU 2005202592	A1	20050707	AU 2005-202592	20050615
PRIORITY APPLN. INFO.:			US 1999-387767 A	19990901
			WO 2000-US23745 W	20000830
			US 2001-781195 A3	20010213

APPLICANTS

OTHER SOURCE(S): MARPAT 134:207821
GI



I

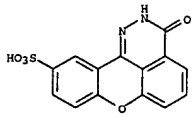


II

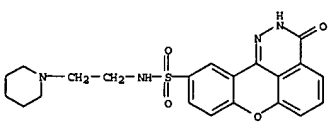
AB Title compds. [I; R = H, lower alkyl; R1 = H, SO3H; m = 0, 1; n = 0, 1; p = 1, 2; Y = CO, O, N; Z = O, S; X = O, S, bond; W = CN, heteoaryl, cycloalkyl; COCH3, SO3H, H; T = alkenylene, arylene, aralkylene, alkarylene, bond; dotted = single, double], pharmaceutically acceptable salt, hydrate, and prodrug are prepared as PARP inhibitors in pharmaceutical compns., and methods of using the disclosed compds. for treating cellular damage, such as neural or cardiovascular tissue damages. Thus, the title compound II was prepared

IT 328525-74-2P 328525-75-3P 328525-76-4P
328525-82-2P 328525-83-3P 328525-84-4P
328525-85-5P 328525-86-6P 328525-87-7P
328525-88-8P 328525-89-9P 328525-90-2P
328525-91-3P 328525-92-4P 328525-93-5P
328525-95-7P 328525-98-0P 328525-99-1P
328526-08-5P 328526-09-6P 328526-12-1P
328526-13-2P 328526-16-5P 328526-17-6P
328526-18-7P 328526-19-8P 328526-21-2P
328526-27-8P 328526-28-9P 328526-29-0P
328526-31-4P 328526-33-6P 328526-34-7P
328526-35-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzopyranodephthalazineonesas PARP inhibitors for treating cellular damages)

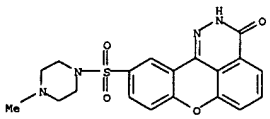
RN 328525-74-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonicacid, 2,3-dihydro-3-oxo- (9CI) (CA INDEX NAME)



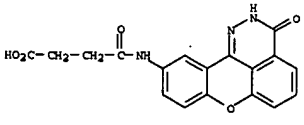
RN 328525-75-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-3-oxo-N-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)



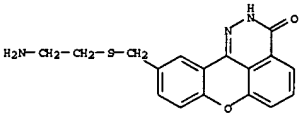
RN 328525-76-4 CAPLUS
CN Piperazine, 1-[(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)sulfonyl]-4-methyl- (9CI) (CA INDEX NAME)



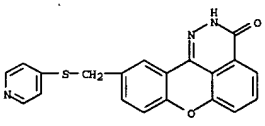
RN 328525-82-2 CAPLUS
CN Butanoic acid, 4-[(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)amino]-4-oxo- (9CI) (CA INDEX NAME)



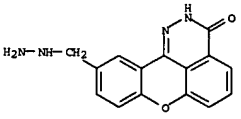
RN 328525-83-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[(2-aminoethyl)thio]methyl]- (9CI) (CA INDEX NAME)



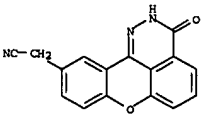
RN 328525-84-4 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(4-pyridinylthio)methyl]- (9CI) (CA INDEX NAME)



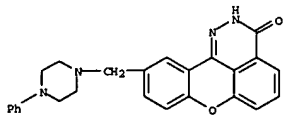
RN 328525-85-5 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(hydrazinomethyl)- (9CI) (CA INDEX NAME)



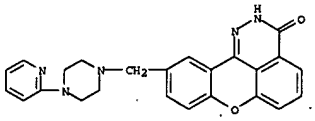
RN 328525-86-6 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-acetonitrile,2,3-dihydro-3-oxo- (9CI) (CA INDEX NAME)



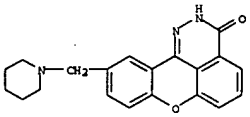
RN 328525-87-7 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(4-phenyl-1-piperazinyl)methyl]- (9CI) (CA INDEX NAME)



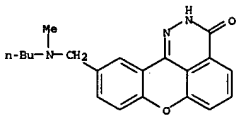
RN 328525-88-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(2-pyridinyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



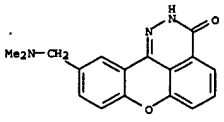
RN 328525-89-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(1-piperidinylmethyl)- (9CI) (CA INDEX NAME)



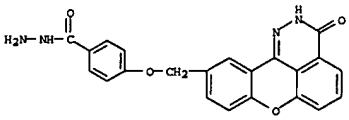
RN 328525-90-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(butylmethylamino)methyl]- (9CI) (CA INDEX NAME)



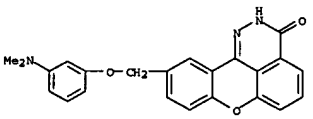
RN 328525-91-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(dimethylamino)methyl]- (9CI) (CA INDEX NAME)



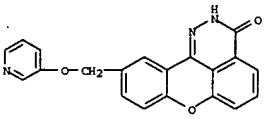
RN 328525-92-4 CAPLUS
CN Benzoic acid, 4-[(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methoxy]-, hydrazide (9CI) (CA INDEX NAME)



RN 328525-93-5 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[3-(dimethylamino)phenoxy]methyl]- (9CI) (CA INDEX NAME)



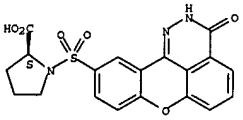
RN 328525-95-7 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[(3-pyridinyloxy)methyl]- (9CI) (CA INDEX NAME)



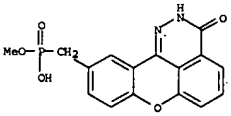
RN 328525-98-0 CAPLUS
CN L-Proline, 1-[(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

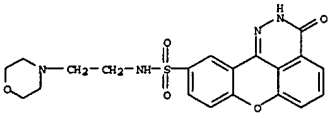
APPLICANTS



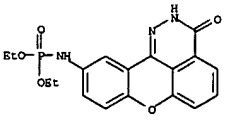
RN 328525-99-1 CAPLUS
CN Phosphonic acid, [(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methyl]-, monomethyl ester (9CI) (CA INDEX NAME)



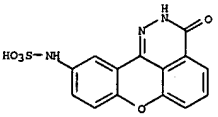
RN 328526-08-5 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-N-[2-(4-morpholinyl)ethyl]-3-oxo- (9CI) (CA INDEX NAME)



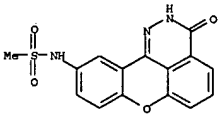
RN 328526-09-6 CAPLUS
CN Phosphoramidic acid, (2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)-, diethyl ester (9CI) (CA INDEX NAME)



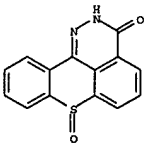
RN 328526-12-1 CAPLUS
CN Sulfamic acid, (2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)- (9CI) (CA INDEX NAME)



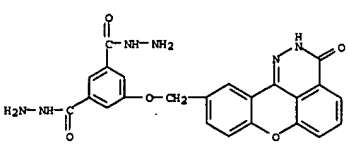
RN 328526-13-2 CAPLUS
CN Methanesulfonamide, N-(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)- (9CI) (CA INDEX NAME)



RN 328526-16-5 CAPLUS
CN [1]Benzothiopyrano[4,3,2-de]phthalazin-3(2H)-one,7-oxide (9CI) (CA INDEX NAME)

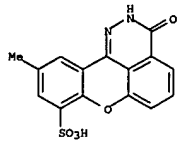


RN 328526-17-6 CAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)methoxy]-, dihydrazide (9CI) (CA INDEX NAME)

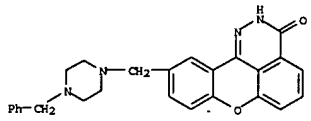


RN 328526-18-7 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-8-sulfonicacid, 2,3-dihydro-10-methyl-

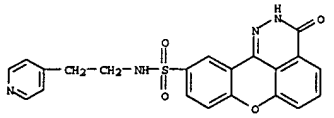
3-oxo- (9CI) (CA INDEX NAME)



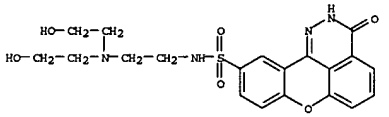
RN 328526-19-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(phenylmethyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



RN 328526-21-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-3-oxo-N-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



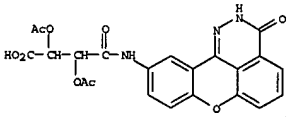
RN 328526-27-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,N-[2-[bis(2-hydroxyethyl)amino]ethyl]-2,3-dihydro-3-oxo-(9CI) (CA INDEX NAME)



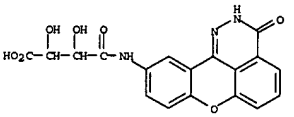
RN 328526-28-9 CAPLUS

APPLICANTS

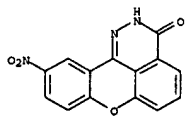
oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)amino]-4-oxo-(9CI) (CA INDEX NAME)



RN 328526-35-8 CAPLUS
CN Butanoic acid, 4-[(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)amino]-2,3-dihydroxy-4-oxo- (9CI) (CA INDEX NAME)

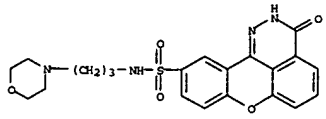


IT 220938-25-0P 220938-26-1P 328525-78-6P
328525-79-7P 328525-80-0P 328525-81-1P
328525-94-6P 328525-96-8P 328525-97-9P
328526-00-7P 328526-02-9P 328526-03-0P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzopyranodephthalazineonesas PARP inhibitors for treating cellular damages)
RN 220938-25-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-nitro- (9CI) (CA INDEX NAME)

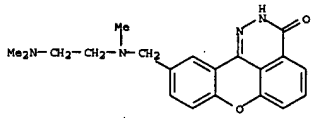


RN 220938-26-1 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-amino- (9CI) (CA INDEX NAME)

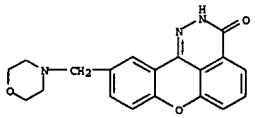
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-N-[3-(4-morpholinyl)propyl]-3-oxo- (9CI) (CA INDEX NAME)



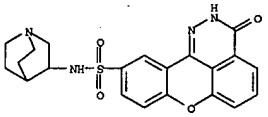
RN 328526-29-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[[2-(dimethylamino)ethyl]methylamino]methyl]-(9CI) (CA INDEX NAME)



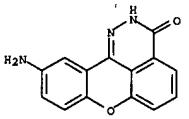
RN 328526-31-4 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(4-morpholinylmethyl)-(9CI) (CA INDEX NAME)



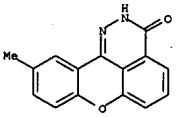
RN 328526-33-6 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,N-1-azabicyclo[2.2.2]oct-3-yl-2,3-dihydro-3-oxo-(9CI) (CA INDEX NAME)



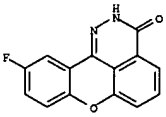
RN 328526-34-7 CAPLUS
CN Butanoic acid, 2,3-bis(acetyloxy)-4-[(2,3-dihydro-3-



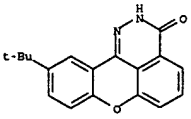
RN 328525-78-6 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-methyl- (9CI) (CA INDEX NAME)



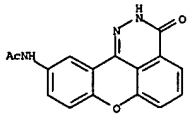
RN 328525-79-7 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-fluoro- (9CI) (CA INDEX NAME)



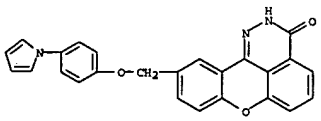
RN 328525-80-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(1,1-dimethylethyl)-(9CI) (CA INDEX NAME)



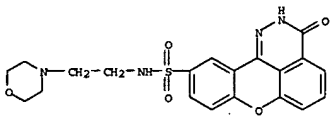
RN 328525-81-1 CAPLUS
CN Acetamide, N-(2,3-dihydro-3-oxo[1]benzopyrano[4,3,2-de]phthalazin-10-yl)-(9CI) (CA INDEX NAME)



RN 328525-94-6 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-[[4-(1H-pyrrol-1-yl)phenoxy]methyl]- (9CI) (CA INDEX NAME)

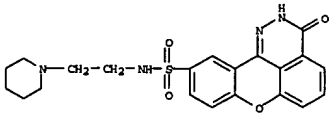


RN 328525-96-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-N-[2-(4-morpholinyl)ethyl]-3-oxo-, monohydrochloride (9CI) (CA INDEX NAME)



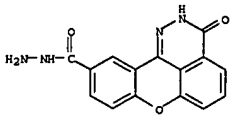
● HCl

RN 328525-97-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-sulfonamide,2,3-dihydro-3-oxo-N-[2-(1-piperidinyl)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

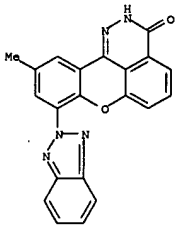


● HCl

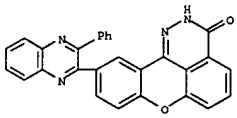
RN 328526-00-7 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazine-10-carboxylicacid, 2,3-dihydro-3-oxo-, hydrazide (9CI) (CA INDEX NAME)



RN 328526-02-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,8-(2H-benzotriazol-2-yl)-10-methyl- (9CI) (CA INDEX NAME)



RN 328526-03-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(3-phenyl-2-quinoxalinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

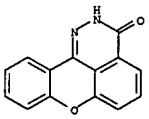
L4 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:184260 CAPLUS
DOCUMENT NUMBER: 130:209323
TITLE: Preparation of PARP inhibitors
INVENTOR(S): Jackson, Paul F.; Li, Jia-He; Maclin, Keith M.; Zhang, Jie
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9911649	A2	19990311	WO 1998-US18185	19980902
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6346536	B1	20020212	US 1997-922548	19970903
US 6635642	B1	20031021	US 1998-145176	19980901
CA 2294074	A1	19990311	CA 1998-2294074	19980902
AU 9893748	A	19990322	AU 1998-93748	19980902
EP 1012153	A1	20000628	EP 1998-946812	19980902
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

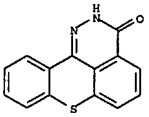
PRIORITY APPLN. INFO.:

US 1997-922520	A	19970903
US 1997-922548	A	19970903
US 1998-79512	A	19980515
US 1998-145176	A	19980901
WO 1998-US18185	W	19980902

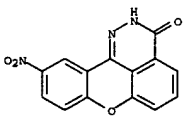
AB PARP inhibitors were prepared and tested for their activity. E.g., 6-(aminocarbonyl)-4-quinolinecarboxylicacid was prepared
IT 220938-23-8P 220938-24-9P 220938-25-0P
220938-26-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of PARP inhibitors)
RN 220938-23-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one(9CI) (CA INDEX NAME)



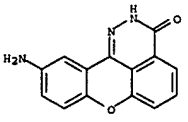
RN 220938-24-9 CAPLUS
CN [1]Benzothiopyrano[4,3,2-de]phthalazin-3(2H)-one(9CI) (CA INDEX NAME)



RN 220938-25-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-nitro- (9CI) (CA INDEX NAME)



RN 220938-26-1 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-amino- (9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:184256 CAPLUS
DOCUMENT NUMBER: 130:209714
TITLE: Tetracyclic heteroaromatic compounds as poly(ADP-ribose) polymerase (PARP) inhibitors for

treating neural or cardiovascular tissue damage

INVENTOR(S): Li, Jia-He; Zhang, Jie; Jackson, Paul F.; Maclin, Keith M.

PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA

SOURCE: PCT Int. Appl., 122 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 17

PATENT INFORMATION:

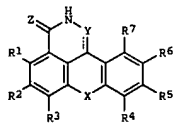
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9911645	A1	19990311	WO 1998-US18189	19980902
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6346536	B1	20020212	US 1997-922548	19970903
US 6306889	B1	20011023	US 1998-47502	19980325
US 6514983	B1	20030204	US 1998-145181	19980901
CA 2294133	A1	19990311	CA 1998-2294133	19980902
AU 9892982	A	19990322	AU 1998-92982	19980902
BR 9812185	A	20000718	BR 1998-12185	19980902
EP 1019409	A1	20000719	EP 1998-945828	19980902
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
HU 200003569	A2	20010730	HU 2000-3569	19980902
JP 2002510332	T	20020402	JP 1999-516974	19980902
NZ 503043	A	20021025	NZ 1998-503043	19980902
NO 2000001001	A	20000405	NO 2000-1001	20000228

PRIORITY APPLN. INFO.:

US 1997-922548	A	19970903
US 1998-47502	A	19980325
US 1998-145181	A	19980901
WO 1998-US18189	W	19980902

OTHER SOURCE(S): MARPAT 130:209714

GI

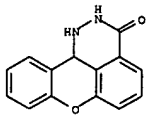


I

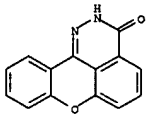
AB Title compds. I [Y = alkylhalo, alkyl-COG, COG, direct bond, CO, O, NR11, CR8; G = NR11R16, OR9, SR9, R10; Z = O, S, NR11; X = NR16, O, S, CR12R13, CO, bond, -CR12CR13, CR12R13CR14R15; R1-R8, R10, R12-R15 = H, halo, alkylhalo, OH, C1-C9 alkyl, C2-C9 alkenyl group, C3-C8 cycloalkyl, C5-C7 cycloalkenyl, aryl, amino, alkylamino, NO2, NO, CO2H, aralkyl; R9 = H, OH, C1-C9 alkyl, C2-C9 alkenyl, C3-C8 cycloalkyl, C5-C7 cycloalkenyl, aryl, NH2, alkylamino, CO2H, aralkyl; R11, R16 = H, halo, alkylhalo, OH, C1-C9 alkyl, C2-C9 alkenyl group, C3-C8 cycloalkyl, C5-C7 cycloalkenyl, aryl, NH2, alkylamino, CO2H, or aralkyl] were prepared for use as PARP inhibitors for treating neural or cardiovascular tissue damage. Thus, I [X, Z = O, Y = NH, R1-R7 = H, the dotted bond is a single bond] was prepared from 9-xanthenecarboxamide by reduction to the amine, conversion to isocyanate, and cyclization and had a PARP-inhibiting IC50 of 0.20μM.

IT 220938-19-2P 220938-23-8P 220938-24-9P
220938-25-0P 220938-26-1P 220938-28-3P
220938-32-9P 220938-35-2P 220938-36-3P
220938-37-4P 220938-39-6P 220938-40-9P
220938-42-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzopyranoisoquinolinones and benzopyranophthalazinones as poly(ADP-ribose) polymerase inhibitors)

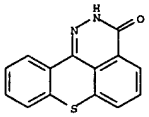
RN 220938-19-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,1,11b-dihydro- (9CI) (CA INDEX NAME)



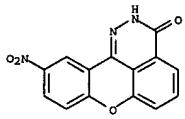
RN 220938-23-8 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one(9CI) (CA INDEX NAME)



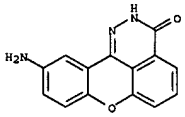
RN 220938-24-9 CAPLUS
CN [1]Benzothiopyrano[4,3,2-de]phthalazin-3(2H)-one(9CI) (CA INDEX NAME)



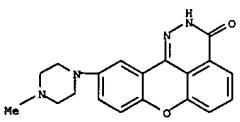
RN 220938-25-0 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-nitro- (9CI) (CA INDEX NAME)



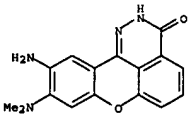
RN 220938-26-1 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-amino- (9CI) (CA INDEX NAME)



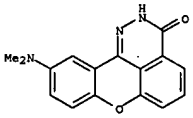
RN 220938-28-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



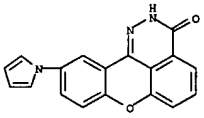
RN 220938-32-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-amino-9-(dimethylamino)- (9CI) (CA INDEX NAME)



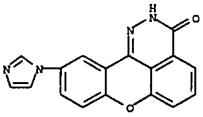
RN 220938-35-2 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(dimethylamino)- (9CI) (CA INDEX NAME)



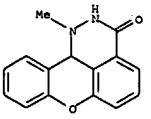
RN 220938-36-3 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(1H-pyrrol-1-yl)- (9CI) (CA INDEX NAME)



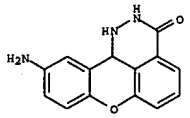
RN 220938-37-4 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-(1H-imidazol-1-yl)- (9CI) (CA INDEX NAME)



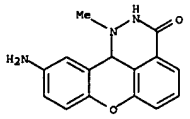
RN 220938-39-6 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,1,11b-dihydro-1-methyl- (9CI) (CA INDEX NAME)



RN 220938-40-9 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-amino-1,11b-dihydro- (9CI) (CA INDEX NAME)

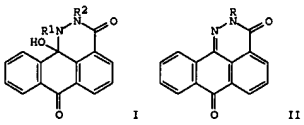


RN 220938-42-1 CAPLUS
CN [1]Benzopyrano[4,3,2-de]phthalazin-3(2H)-one,10-amino-1,11b-dihydro-1-methyl- (9CI) (CA INDEX NAME)

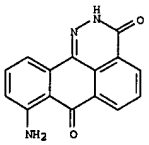


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

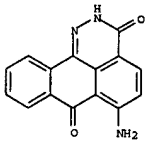
L4 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:509328 CAPLUS
DOCUMENT NUMBER: 89:109328
TITLE: Structure and reactions of N,N'-dialkylhydrazides of anthraquinone-1-carboxylic acid
AUTHOR(S): Mednis, J.
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR
SOURCE: Tezisy Dokl. - Resp. Konf. Molodykh Uch.-Khim., 2nd (1977), Volume 1, 3-4. Akad. Nauk Est. SSR, Inst. Khim.: Tallinn, USSR.
CODEN: 38RMAG
DOCUMENT TYPE: Conference
LANGUAGE: Russian
GI



AB Treatment of I (R1 = R2 = Me, R1R2 = o-H2CC6H4CH2) with SOCl2 or HCl under mild conditions gave II (R = Me, o-C6H4CHO).
IT 53453-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thionyl chloride and hydrochloric acid)
RN 53453-78-4 CAPLUS

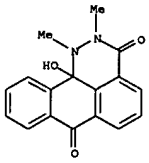


RN 57981-27-8 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-amino- (7CI, 9CI) (CA INDEX NAME)

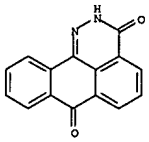


L4 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:3986 CAPLUS
DOCUMENT NUMBER: 84:3986
TITLE: Infrared absorption spectra and structure of oxazon- and pyridazonanthrone and their derivatives
AUTHOR(S): Zaitsev, B. E.; Mikhailova, T. A.; Fain, V. Ya.
CORPORATE SOURCE: Nauchno-Issled. Inst. Org. Poluprod. Krasitelei, Moscow, USSR
SOURCE: Zhurnal Fizicheskoi Khimii (1975), 49(9), 2194-9
CODEN: ZFKHA9; ISSN: 0044-4537
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB The ir data for I (X = O, NH, NPh, NC6H4Br-p, NC6H4NO2-p; R, R1 = H, NH2) and related compds. indicated that the dioxo forms predominate. In I (R or R1 = NH2), H bonding exists between the NH2 group and the carbonyl O; the stability of the H bond is greater when R = NH2.
IT 731-37-3 57449-83-9
RL: PRP (Properties)
(ir spectrum of)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)

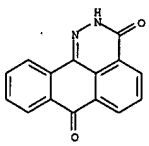
CN 1H-Dibenzo[de,h]cinnoline-3,7(2H,11bH)-dione,11b-hydroxy-1,2-dimethyl-(9CI) (CA INDEX NAME)



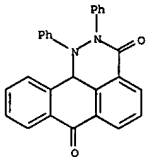
L4 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:42754 CAPLUS
DOCUMENT NUMBER: 84:42754
TITLE: Electron absorption spectra and structure of pyridazonanthrone and its amino derivatives
AUTHOR(S): Zaitsev, B. E.; Mikhailova, T. A.; Fain, V. Ya.
CORPORATE SOURCE: USSR
SOURCE: Zhurnal Fizicheskoi Khimii (1975), 49(10), 2552-5
CODEN: ZFKHA9; ISSN: 0044-4537
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB The long-wavelength band in the electronic absorption spectrum of I was assigned to an $S_{n\pi^*}$ transition involving charge transfer from the pyridazone ring to the anthrone ring. The analogous band for the 4-amino, 5-amino, and 5-amino-N-phenyl derivs. was assigned to an $S_{2p\pi^*}$ transition involving charge transfer from the amino N to the ring π system. Atomic charge densities were calculated
IT 731-37-3 57981-26-7 57981-27-8
RL: PRP (Properties)
(uv-visible spectrum of, solvent effect on)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



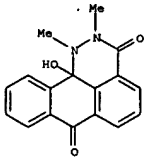
RN 57981-26-7 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-amino- (7CI, 9CI) (CA INDEX NAME)



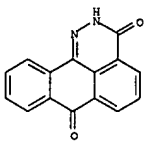
RN 57449-83-9 CAPLUS
CN 1H-Dibenzo[de,h]cinnoline-3,7(2H,11bH)-dione,1,2-diphenyl- (9CI) (CA INDEX NAME)



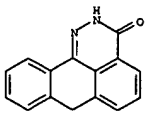
L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:520557 CAPLUS
DOCUMENT NUMBER: 81:120557
TITLE: Effect of the rigid conformation of thecarbonyl group on ring-chain isomerism of anthraquinone-1-carboxylic acid derivatives
AUTHOR(S): Valters, R.; Mednis, J.
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1974), 10(6), 1248-52
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Anthraquinonecarboxamides (I; R = H, Me, Et, Me2CH, Ph, NMe2) were obtained in 22-63% yields by amination of anthraquinone-1-carbonyl chloride (II) with RNH2. Treatment of II with MeNHNH2 in Et3N gave dibenzocinnoline (III).
IT 53453-78-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53453-78-4 CAPLUS
CN 1H-Dibenzo[de,h]cinnoline-3,7(2H,11bH)-dione,11b-hydroxy-1,2-dimethyl-(9CI) (CA INDEX NAME)



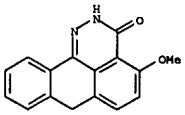
L4 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:111797 CAPLUS
DOCUMENT NUMBER: 74:111797
TITLE: Anthracenes from benzyl furans
AUTHOR(S): Mavoungou-Gomes, Louis
CORPORATE SOURCE: Fac. Libre Sci., Angers, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1971), 272(7), 687-90
CODEN: CHDCAQ; ISSN: 0567-6541
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB The anthrone I was prepared by treating the adduct from 2-benzylfuran and MeO2CC.tplbond.CO2Me with BF3, methylating the phenolic OH of 4,2,3-PhCH2(MeO2C)2-C6H2OH, saponification and dehydration to the anhydride, and cyclization with AlCl3. I and II were lactonized with Ac2O, converted to dibenzo[c,d,g]indoles with amines, or converted to 7H-dibenzo[d,e,h]cinnolines with hydrazines. The dibenzocinnolines showed no tautomerism. Cr2O3 oxidation of II gave 1-carboxyanthraquinone. 2-Oxo-4,5-dihydro-2H-anthra[9,1-bc]-furanwas similarly prepared from the adduct of 2-benzylfuran with maleic anhydride.
IT 731-37-3P 31272-82-9P 31272-83-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



RN 31272-82-9 CAPLUS
CN 3H-Dibenzo[de,h]cinnolin-3-one,2,7-dihydro- (8CI) (CA INDEX NAME)



RN 31272-83-0 CAPLUS
CN 3H-Dibenzo[de,h]cinnolin-3-one,2,7-dihydro-4-methoxy- (8CI) (CA INDEX NAME)



L4 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:51639 CAPLUS
DOCUMENT NUMBER: 62:51639
ORIGINAL REFERENCE NO.: 62:9129e-h
TITLE: Pyridazoanthrone and its derivatives. III. Oxazoanthrone and its connection with pyridazoanthrone
AUTHOR(S): Dokunikhin, N. S.; Fain, V. Ya.
CORPORATE SOURCE: Res. Inst. Org. Intermed. and Dyes, Rubezhnoe
SOURCE: Zhurnal Obshchei Khimii (1964), 34(11), 3769-71
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB cf. CA 62, 4027e. Oxazoanthrone (I) (cf. Ullmann and van der Schalk, Ann. 388, 199(1912)) heated in AcOH with N2H4 6 hrs. gave 30.1% pyridazoanthrone, m. 425-6°. Similarly, PhNHNH2 gave N-phenylpyridazoanthrone (II), m. 290.3-1.0°. I heated with Br in AcOH in a sealed tube 2.5 hrs. at 150° gave after an aqueous treatment anthraquinone-1-carboxylic acid, m. 292-3°. I refluxed with 98% HNO3 gave the same acid in 88% yield. 4-Aminoanthraquinone-1-carboxylic acid refluxed 0.5 hr. with aqueous KOAc and HONH2.H2SO4, then with aqueous NH4OH, gave on acidification 78.3% 4-aminooxazoanthrone, decomposed 291°. Similarly was prepared 83.3% 5-aminooxazoanthrone, decomposed 283°. Anthraquinone-1,4-dicarboxylic acid refluxed as above with HONH2.H2SO4 gave anthra-1,9(N),10(N),4-dioxazone(III), decomposed 318-19°. Spectral data (uv) on these products were reported.
IT 731-37-3P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione
RL: PREP (Preparation)
(preparation of)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)

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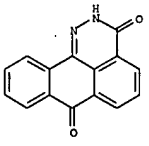
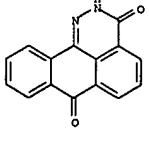
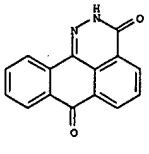


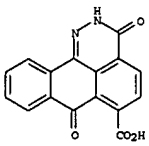
L4 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:51638 CAPLUS
DOCUMENT NUMBER: 62:51638
ORIGINAL REFERENCE NO.: 62:9129d-e
TITLE: Ion exchangers with complex-forming anchor groups. XII. Existence of ethylenediaminetriacetic acid
AUTHOR(S): Kuehn, G.; Hoyer, E.; Hering, R.
CORPORATE SOURCE: Karl-Marx-Univ., Leipzig, Germany
SOURCE: Zeitschrift fuer Chemie (1964), 4(12), 462-3
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German
AB cf. CA 60, 1142g. Me 1-aziridinylacetate (9.5 g.) and 35 g. (EtO2CCH2)2NH was heated 25 hrs. at 80° in 45 ml. alc. with a few drop alc. HCl to give 40% the Me Et (I) ester of 2-oxopiperazine-N,N'-diaceticacid, b0.001 143-5°, n20D 1.4813. Saponification of I with Ba(OH)2 gave the lactam of ethylenediaminetriaceticacid, 2-oxopiperazine-N,N'-diacetic acid (II), decomposed 214-15°. The 1:1 Cu2+ complex of II with 3 moles H2O crystallized in fine light blue needles from a solution of II and CuNO3; at 120°, 2 moles H2O were lost and the other mole was lost at 135-40°. Titration curves and stability consts. of the acid and the Ca2+, Cu2+, and Ni2+ complexes shows the inductive effect of the oxo group makes II more acid than piperazine-N,N'-diaceticacid.
IT 731-37-3P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione
RL: PREP (Preparation)
(preparation of)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



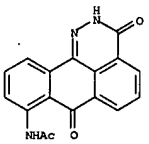
L4 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:22573 CAPLUS
DOCUMENT NUMBER: 62:22573
ORIGINAL REFERENCE NO.: 62:4027d-h,4028a
TITLE: Pyridazoanthrone and its derivatives. II. N-Arylpyridazoanthrones
AUTHOR(S): Dokunikhin, N. S.; Fain, V. Ya.
CORPORATE SOURCE: Res. Inst. Org. Intermed. and Dyes, Rubezhnoe
SOURCE: Zhurnal Obshchei Khimii (1964), 34(10), 3354-9
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. CA 55, 24699a; 61, 9493b. Refluxing anthra[9,1-cd]pyridazine-2,6-dione with the appropriate halo compound in PhNO2 in the presence of KOAc, powdered Cu, and Cu(OAc)2 10 hrs. gave 1-arylanthra[9,1-cd]pyridazine-2,6-diones (aryl group shown): 72% Ph (I), m. 287.6-89°; p-O2NC6H4, 68.7%, m. 367-8° (o-isomer, 67.3%, m. 266.7-8.3°); 2,4-(O2N)2C6H3, 84.7%, m. 314-14.8°; 1-anthraquinolyl, 78.8%, m. 338-9°; 4-methyl-1-anthraquinonyl, 78.5%, m. 367-8°; 3-benzanthronyl, 77.2%, m. 380-1°. Similarly prepared were 4',7-dinitro-1-phenylanthra[9,1-cd]pyridazine-2,6-dione,21.3%, m. 372-4°; and its ,2'7-dinitro analog, 17%, m. 285-6.5°. Refluxing 4-aminoanthraquinone-1-carboxylicacid with PhNHNH2 in 50% AcOH and NaOAc 0.5 hr. gave 60% yellow 5-amino-1-phenyl-anthra[9,1-cd]pyridazine-2,6-dione, m. 338.6-9.8°; this was formed similarly in 78.8% yield from 4-nitroanthraquinone-1-carboxylicacid. Refluxing anthraquinone-1-carboxylicacid in PhCl with PCl5 1 hr., followed by further heating 1 hr. with added p-O2NC6H4NHNH2 gave 40.2% yellow 1-(p-nitrophenyl)anthra-[9,1-cd]pyridazine-2,6-dione(II), m. 362-4°; the same was formed in 26.9% yield after similar reaction in 60% AcOH-KOAc solution without PCl5; or by the nitration of I with 98% HNO3 in concentrated H2SO4 1 hr. at 0-5°. Similarly was prepared 55.7% 1-(o-nitrophenyl)anthra[9,1-cd]pyridazine-2,6-dione,m. 265-6°; and 82.7% 1-(2,4-dinitrophenyl)anthra[9,1-cd]pyridazine-2,6-dione, m. 313-14.3°. Nitration of I with mixed acid as above gave 100% 4',7-dinitro derivative, m. 381-2°, also formed from the 7-nitro derivative of I and p-ClC6H4NO2; the reaction also gave an isomeric dinitro derivative, m. 319.7-20°. II was reduced with Na2S in aqueous EtOH in 4 hrs. to the p-aminophenyl analog, 83.6%, m. 317.8-19.2°; similarly was prepared 76.3% orange o-aminophenyl analog, m. 338-8.8°; and 100% red-brown 2,4-diaminophenyl analog, m. 329.5-31.3°. Anthraquinone-1,4-dicarboxylicacid and PhNHNH2 in 50% AcOH in the presence of KOAc refluxed 2 hrs. gave 60% 1,6-diphenylanthrabis[9,1-cd:10,4,c'd']pyridazine-2,6-dione(III), m. 381-2°, but with larger proportions of the dicarboxylic acid, the reaction gave 74% 1-phenylanthra[9,1-cd]pyridazine-2,6-dione-5-carboxylicacid, m. 388-9°. Bromination of I in AcOH, finally at reflux 2 hrs., gave 73.2% yellow 1-(p-bromophenyl)anthra[9,1-cd]pyridazine-2,6-dione,m. 308.5-9.3°.
IT 731-37-3, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione
(derivs.)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



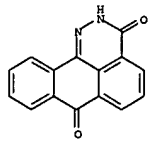
L4 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:454842 CAPLUS
DOCUMENT NUMBER: 61:54842
ORIGINAL REFERENCE NO.: 61:9494a-c
TITLE: Transformation of 3-hydrazinopyridazino[4,5,6-m,l]fluorene
AUTHOR(S): Dokunikhin, N. S.; Mikhalenko, S. A.
SOURCE: Zhurnal Obshchei Khimii (1964), 34(7), 2473-4
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB 3-Chloropyridazino[4,5,6-m,l]fluoreneand N2H4.H2O gave the 3-hydrazino analog, isolated as the hydrate (I), which with HgO in alc. NaOH gave 80% pyridazino[4,5,6-m,l]fluorene (II), m. 123.6-25°; in the absence of HgO the yield was 54%. I, decomposed 255.6-56°, and 2 moles aqueous CuSO4 gave 85% 1-cyanofluorenone, m. 180-80.5°, also formed in 10% yield in alc. NaOH. Saponification with alc. alkali gave fluorenone-1-carboxylic acid. Similarly, 3-hydrazino-9-methylpyridazino[4,5,6-m,l]fluorene hydrate, m. 277.5-8.6°, gave 60% 1-cyano-7-methylfluorenone, m. 209.1-10°. I was unchanged by oxidizing agents such as Na2AsO4. II picrate decomposed 221-2°.
IT 97594-69-9P, 3H-Dibenzo[de,h]cinnoline-6-carboxylicacid, 2,7-dihydro-3,7-dioxo 98000-26-1P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione, 8-acetamido-
RL: PREP (Preparation)
(preparation of)
RN 97594-69-9 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-6-carboxylicacid, 2,7-dihydro-3,7-dioxo- (7CI) (CA INDEX NAME)



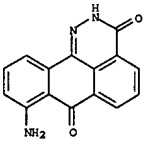
RN 98000-26-1 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-acetamido- (7CI) (CA INDEX NAME)



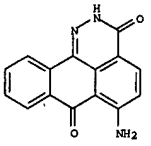
L4 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:454841 CAPLUS
DOCUMENT NUMBER: 61:54841
ORIGINAL REFERENCE NO.: 61:9493f-h,9494a
TITLE: Pyridazoneanthrone and its derivatives I
AUTHOR(S): Dokunikhin, N. S.; Fain, V. Ya.
SOURCE: Zhurnal Obshchei Khimii (1964), 34(7), 2372-4
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Refluxing anthraquinone-1-carboxylicacid in aqueous NaOAc in the presence of N2H4.H2SO4 7 hrs. gave 93% pyridazoneanthrone (I, R = H) (II), m. 426-7°; simple heating of the acid with N2H4.H2O 3 hrs. gave a 92.5% yield. Similar reaction of 4-aminoanthraquinone-1-carboxylicacid gave 85.7% 4-aminopyridazoneanthrone, decomposed 351.5-2.8°, also formed in 74.6% yield from 4-nitroanthraquinone-1-carboxylicacid refluxed 1 hr. with PCl5 in C6H6, then treated in the cold with N2H4.H2O 1 hr., followed by refluxing with dilute NH4OH; the use of N2H4.H2SO4 gave an 82.7% yield. II nitrated in concentrated H2SO4 with 98% HNO3 at 0° 1 hr. gave I (R = NO2), decomposed 291.2-3°, which with aqueous Na2S 1.5 hrs. at reflux gave 89% I (R = NH2), decomposed 372-3°, also formed in 91.5% yield from 5-aminoanthraquinone-1-carboxylicacid, via the route used above for preparation of II. I (R = NH2) was also formed by treatment of 5-nitroanthraquinone-1-carboxylicacid with PCl5 and N2H4, as shown above, the yield being 70.2%. The amine heated with Ac2O 0.5 hr. gave I (R = AcNH), decomposed 370-1°. Anthraquinone-1,4-dicarboxylicacid (III) heated successively with PCl5, then N2H4.H2O gave 92.5% anthra-1,4-dipyridazone (IV), decomposed about 500°. III in hot aqueous NaOAc was treated with N2H4.H2SO4 and refluxed 3 hrs. to yield 4% insol. IV, and 93.6% pyridazoneanthrone-4-carboxylicacid, decomposed 333.5-4.8°.
IT 731-37-3P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione 57981-26-7P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-amino- 57981-27-8P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-amino- 97216-39-2P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-nitro- 97594-69-9P, 3H-Dibenzo[de,h]cinnoline-6-carboxylicacid, 2,7-dihydro-3,7-dioxo 98000-26-1P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione, 8-acetamido-
RL: PREP (Preparation)
(preparation of)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



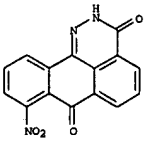
RN 57981-26-7 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-amino- (7CI, 9CI) (CA INDEX NAME)



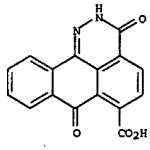
RN 57981-27-8 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-amino- (7CI, 9CI) (CA INDEX NAME)



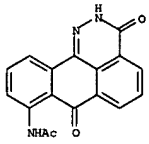
RN 97216-39-2 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-nitro- (7CI) (CA INDEX NAME)



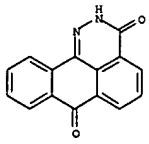
RN 97594-69-9 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-6-carboxylicacid, 2,7-dihydro-3,7-dioxo- (7CI) (CA INDEX NAME)



RN 98000-26-1 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-acetamido- (7CI) (CA INDEX NAME)



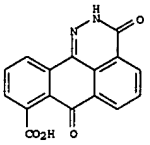
L4 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:454840 CAPLUS
DOCUMENT NUMBER: 61:54840
ORIGINAL REFERENCE NO.: 61:9493e-f
TITLE: Action of nitric acid on polybromophenothiazines
AUTHOR(S): Bodea, Cornel; Farcasan, V.; Oprean, I.
CORPORATE SOURCE: Chem. Inst., Cluj, Rom.
SOURCE: Zhurnal Obshchei Khimii (1964), 34(7), 2369-71
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 55, 550b. Nitration of polybromophenothiazine-5,5-dioxidesin fuming HNO3 with ice cooling, followed by 12 hrs. at room temperature, gave the following products: 1,9-dibromo-3,7-dinitrophenothiazine5,5-dioxide, m. 305°, formed from 1,3,7,9-tetrabromophenothiazinedioxide or 1,3,7,9-tetrabromophenothiazine; 1,3,7,9-tetranitrophenothiazine 5,5-dioxide, m. 344-5°, formed from 3,7-dibromophenothiazine 5,5-dioxide, or 3,7-dibromophenothiazine; 1-bromo-3,7,9-trinitrophenothiazine5,5-dioxide, m. 311-12°, formed from 1,3,7-tribromophenothiazine5,5-dioxide or 1,3,7-tribromophenothiazine; 1-nitro-3,7-dibromophenothiazine5,5-dioxide, m. 297-8°, formed from 3,7-dibromophenothiazine5,5-dioxide by heating with fuming HNO3 in AcOH 2 min. at reflux.
IT 731-37-3P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione
RL: PREP (Preparation)
(preparation of)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



L4 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:67720 CAPLUS
DOCUMENT NUMBER: 55:67720
ORIGINAL REFERENCE NO.: 55:12867e-i,12868a-d
TITLE: Anthradipyridazones and their use in polymeric materials as optical bleaching agents
INVENTOR(S): Irving, Francis; Reece, Charles H.; Munro, Neil; Wilson, Robert H.
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 838994		19600622	GB 1956-37142	19561205
DE 1060403			DE	
US 2992220		19610711	US 1957-699440	19571129

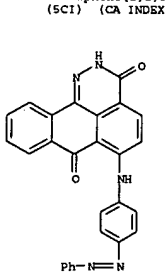
GI For diagram(s), see printed CA Issue.
AB Anthra-1'9'(N),10',(N),4'(or5')-dipyridazones of the general formula I, where X and Y are H or univalent organic radicals, are useful as optical bleaching agents for high polymers such as poly(ethylene terephthalate), poly(hexamethyleneadipamide), polycaprolactam, and cellulose acetate. The bleaching agents may be added to the polymer which is then melted and cast or spun, or the compds. may be mixed with the monomers prior to polymerization as in the case of poly(ethylene terephthalate). For example, 2 parts 2-butyl-anthra-1',9'(N)-pyridazone-5'-carboxylicacid (II) and 1 part 2,6-Me2C6H3NH NH2 were heated at 220° for 30 min., cooled, stirred with 100 parts boiling 1% aqueous NaOH, filtered, the precipitate stirred with 100 parts 1% HCl, and filtered to give pale yellow 2-(2,6-dimethylphenyl)-8-butylanthra-1',9'(N),10'-(N),5'-dipyridazonem. 198-200° (EtOH). 1,5-Anthraquinonedicarboxylicacid (10 parts), 3 parts BuNHNH2, and 1.3 parts NaOH were heated at 200° for 15 min., cooled, stirred with 200 parts boiling 1% aqueous NaOH, filtered, 20 parts NaCl added to the filtrate, filtered, the precipitate dissolved in 300 parts H2O, and acidified to precipitate II, m. 250°. Similarly prepared were the following agents and intermediates (color and m.p. given): 2-(2,6-dimethylphenyl)anthra-1',9'(N)-pyridazone-5'-carboxylicacid, pale yellow, 310-12°; 2,8-diphenylanthra-1',9'(N),10'(N),5'-dipyridazone, greenish yellow, 391-3° [o-Cl2C6H4 (III)]; 2,8-di-p-tolylanthra-1',9'(N),10'(N),5'-dipyridazone,-, <390°; 2,8-bis(2-chlorophenyl)anthra-1',9'(N),10'(N),5'-dipyridazone pale yellow 400°; 2,8-bis(2,5-dichlorophenyl)anthra-1',9'(N), 10'(N),5'-dipyridazone, pale yellow, 432°; 2,8-dibutyl-anthra-1',9'(N),10'(N),5'-dipyridazone,yellow, 185-6° (EtOH); 2,7-diphenylanthra-1',9'(N),10'(N),4'-dipyridazone,light greenish yellow, 394.5-6° (III); anthra-1',9'(N),10'(N),5'-dipyridazone,light brown, >400°; 2,8-bis(2,6-dimethylphenyl)anthra-1',9'(N),10'(N),5'-dipyridazone, light yellow, 369° (III); 2,8-bis(2-hydroxyethyl)anthra-1',9'(N),10'(N),5'-dipyridazone,yellow, 307° (III); 2-(2,6-dimethylphenyl)anthra-1',9'(N),10'(N),5'-dipyridazone-, 348-50° (III); 2,8-bis(2,6-diethylphenyl)anthra-1',9'(N),10'(N),5'-dipyridazone, pale yellow, 362°; 2-(2,6-diethylphenyl)anthra-1',9'(N),10'(N),5'-dipyridazone,-, 300°; 2,8-bis(o-bromophenyl)anthra-1',9'(N),10'(N),5'-dipyridazone,cream, -; 2-(6-chloro-2-methylphenyl)anthra-1',9'(N),10'(N),5'-dipyridazone, -, 349°; 2-(6-chloro-2-methylphenyl)anthra-1',9'(N)-pyridazone-5'-carboxylic acid, pale yellow, 305°; 2-(2,6-dichlorophenyl)anthra-1',9'(N),10'(N),5'-dipyridazone,yellow, 379° (III); 2-(2,6-dichlorophenyl)anthra-1',9'(N)-pyridazone-5'-carboxyliacid, pale gray, 325°; anthra-1',9'(N)-pyridazone-5'-carboxylicacid, yellow, 389°; 2-(2,6-dimethylphenyl)-7-butylanthra-1',9'(N)10'(N),4'-dipyridazone, pale yellow, 240-2°; 2-(2,6-dimethylphenyl)-anthra-1',9'(N)-pyridazone-4'-carboxylicacid, yellow, 283-7°; 2,7-dibutylanthra-1',9'(N),10'(N),4'-dipyridazone,pale yellow, 183° (III); 2,7-bis(o-chlorophenyl)anthra-1',9'(N),10'(N),4'-dipyridazone, pale cream, 412-14°; and 2,7-bis(2,6-dimethylphenyl)anthra-1',9'(N),10'(N),4'-dipyridazone, pale yellow, 358°.
IT 132647-76-8, 7H-Dibenzo[de,h]cinnoline-8-carboxylicacid, 2,3-dihydro-3,7-dioxo-
RL: PREP (Preparation)
(preparation of)
RN 132647-76-8 CAPLUS
CN 7H-Dibenzo[de,h]cinnoline-8-carboxylicacid, 2,3-dihydro-3,7-dioxo- (6CI) (CA INDEX NAME)



L4 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1949:45334 CAPLUS
DOCUMENT NUMBER: 43:45334
ORIGINAL REFERENCE NO.: 43:8165f-i,8166a-c
TITLE: Orange anthrapyridazone dyes for wool
INVENTOR(S): Coffey, Samuel; Schofield, Kenneth; Slinger, Frank H.; Tatum, Wm. W.
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

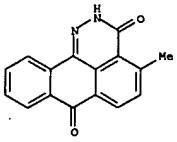
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 615837		19490112	GB 1946-24125	19460814

GI For diagram(s), see printed CA Issue.
AB Anthrapyridazone dyes (I) having the structure shown below, in which X is H or an aryl radical and R is the residue of an azobenzene, are prepared by condensing halogen derivs. of pyridazones with aminoazobenzenes and sulfonating the resulting products. The I are fast and dye wool in orange to orange-red shades. A I is prepared by condensing 6-chloro-2-phenyl-1',9'-anthrapyridaz-3-one (II) with p-aminoazobenzene (III) in the presence of KOAc and Cu bronze in PhNO2, and sulfonating the resulting 6-(p-phenylazoanilino)-2-phenyl-1',9'-pyridaz-3-one. Other I are similarly prepared by sul fonating 6-[p-(p-aminophenylazo)anilino]-2-phenyl-1',9'-anthrapyridaz-3-one (prepared by condensing II with 4,4'-diaminoazobenzene), 6-[p-(p-methoxyphenylazo)anilino]-2-phenyl-1',9'-anthrapyridaz-3-one (prepared by condensing II with 4'-methoxy-4-aminoazobenzene), 6-[p-(4-chloro-2-nitrophenylazo)anilino]-2-phenyl-1',9'-anthrapyridaz-3-one (prepared by condensing II with 4'-chloro-2'-nitro-4-aminoazobenzene), 6-p-phenylazoanilino-2-(p-nitrophenyl)-1',9'-anthrapyridaz-3-one (prepared by condensing 6-chloro-2-(p-nitrophenyl)-1',9'-anthrapyridaz-3-one (IV) with III), 6-p-phenylazoanilino-2-(2,5-dichlorophenyl)anthrapyridaz-3-one (prepared by condensing 6-chloro-2-(2,5-dichlorophenyl)-1',9'-anthrapyridaz-3-one (V) with III), or 6-p-phenylazoanilino-1',9'-anthrapyridaz-3-one (prepared by condensing 6-chloroanthrapyridazone with III. IV is prepared by heating 1-chloroanthraquinone-4-carboxylicacid (VI) and p-nitrophenylhydrazine in EtOH. V is prepared by heating VI with 2,5-dichlorophenylhydrazine in EtOH.
IT 858031-47-7, 7H-Naphtho[1,2,3-de]phthalazine-3,7-(2H)-dione, 6-(p-phenylazoanilino)-
(dye from)
RN 858031-47-7 CAPLUS
CN 7H-Naphtho[1,2,3-de]phthalazine-3,7-(2H)-dione,6-(p-phenylazoanilino)- (5CI) (CA INDEX NAME)



L4 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1929:40448 CAPLUS
DOCUMENT NUMBER: 23:40448
ORIGINAL REFERENCE NO.: 23:4695f-i,4696a-e
TITLE: Anthrahydroquinol-α-carboxylic lactones
AUTHOR(S): Scholl, Roland; Renner, Fritz; Bottger, Oskar; Hass, Sigfrid; Meyer, H. Kurt
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1929), 62B, 1278-95
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C. A. 23, 2710. In addition to the 2 methods described in the earlier papers (treatment of anthrahydroquinol-α-carboxylic acids with Ac2O and of anthraquinone-α-carboxylic anhydrides with Na2S2O4 alone or in the presence of dilute NH4OH or AcOH), anthrahydroquinol-1-carboxylic lactone (I) and its 2-Me derivative (II) have been prepared by the following methods: (1) Short heating of the anthraquinone acids with Zn dust and AcOH in the presence of Ac2O. (2) Reduction of the esters of the quinone acids with acid or alkaline reducing agents. The aryl esters are readily reduced by Na2S2O4 or Zn dust and NH4OH, best by Zn dust and boiling AcOH. Of the alkyl esters, only those of the 2,1-C6H4(CO)2C2H2MeCO2H (III) react in this way; those of the unmethylated C6H4(CO)2C6H3CO2H (IV) are converted exclusively into the hydroquinol acid. (3) From the acid chlorides with Na2S2O4 and NaOH. (4) From the acid amides with Na2S2O4 and very dilute NaOH or AcOH. The methods involving alkalies or NH4OH are not practical as the alkaline solns. of the lactones are very unstable and sensitive to the air. The lactones, themselves red, disiolve easily in aqueous NH4OH, less readily, in NaOH and Na2CO3, with vivid pure blue color and are reppld. red by including CO2; in the blue alkaline solns. they change more or less rapidly, by addition of H2O, into the red anthrahydroquinolcarboxylates; in the NH4OH solns. into the anthrahydroquinolcarboxamides. In C5H5N, I dissolves with its own red color and on cooling seps. from a hot concentrated solution as a red homopolar compound III.C5H5N, but if H2O is added to the red solution it becomes deep blue with formation of the heteropolar true pyrdinium salt which is dissociated back into the red form by heat or much C5H5N. The lactones are sensitive to air in alkaline, acid or neutral solution, especially in C6H6 or xylene in the light. Typical oxidizing agents (PbO2, FeCl3, K3Fe(CN)4, Br, KMnO4) oxidize them more or less rapidly at room temperature; for practical purposes hot PhNO3 is best. II in all cases gave chiefly 2,2'-dimetyl-9,9'-dihydroxy-9,9'-bianthronyl-1,1'-dicarboxylidilactone (V). The oxidation with KMnO4 in Me2CO-AcOH and with Br in C5H5N is instantaneous and quant. and may be used to titrate the lactones. V is also formed from the acid chloride of III in C6H6 with finely divided Ag or PhNMe2. Concentrated H2SO4 decomps. V into III. Zn dust and AcOH, Na2S2O4 and NH4OH very slowly, reduce V to the monomeric II. Aqueous and especially alc. alkalies dissociate V with formation of an olive-green solution containing the salts of the anthraquinone and the anthrahydroquinol acids apparently in quinhydrone-like combination. Probably the primary process is a radical dissociation into an anthroxyl with univalent O. Exposure of V in AcOH to ultra-violet light and heating in certain organic solvents apparently also brings about a similar dissociation I, brown-red, decolorizes above 175° and begins to sublime. Ph ester of IV, m. 213°. 10-Acetate of I, from IV and Zn dust in boiling Ac2O, m. 196°. Me ester of III, light yellow, m. 178-9°; Et ester, m. 144°; Ph ester, pale yellow, m. 218-9° (2-methylpyridazonanthrone, from the Ph ester and N2H4.H2O in boiling C6H6, yellow, m. 332°); p-bromophenyl ester, yellowish, m. 226°. 2-Methylanthrahydroquinol-1-carboxylic acid is precipitated as a yellow jelly from the alkaline Na2S2O4 vat of III. The lactone (II), red, becomes lighter about 235°, m. around 265°, (decomposition). Amide of III from II allowed to stand in NH4OH and then shaken with air, or from the chloride of III in C6H6 with NH3, begins to sinter 255°, darkens 260°, decomps completely at higher temps. Acetate of II, orange, m. 238°. 2,2'-Di-Me homolog of V, turns brown on rapid heating about 270°, m. around 290° (decomposition). It had been concluded, from the work on the quinone anhydrides, that the latter have the normal structure C6H4(CO)2C5H3COR and not the ps-structure C6H4. Since in the reduction of the free quinone acid (III) to II the intermediate hydroquinol acid has been isolated and the amide is reppld. unchanged by air from its alkaline vat, it is concluded that the free anthraquinone-carboxylic acids and their amides likewise have the normal structure, and the same is shown for the esters in the following abstract
IT 858020-37-8, 7-Naphtho[1,2,3-de]phthalazine-3,7(2)-dione, 4-methyl-
RL: PREP (Preparation)

(preparation of)
RN 858020-37-8 CAPLUS
CN 7-Naphtho[1,2,3-de]phthalazine-3,7(2)-dione,4-methyl- (3CI) (CA INDEX NAME)



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DICTIONARY FILE UPDATES: 24 JAN 2007 HIGHEST RN 918400-64-3

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http://www.cas.org/ONLINE/UG/regprops.html

=>
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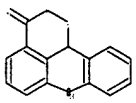
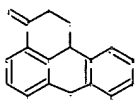




chain nodes :
19
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 22
chain bonds :
3-19
ring bonds :
1-2 1-6 1-7 2-3 2-10 3-4 4-5 5-6 6-11 7-8 7-22 8-9 9-10 11-12 11-13 12-16 12-22 13-14 14-15 15-16
exact/norm bonds :
1-2 1-6 1-7 2-3 3-4 3-19 4-5 5-6 6-11 7-8 7-22 11-12 11-13 12-16 12-22
normalized bonds :
2-10 8-9 9-10 13-14 14-15 15-16
isolated ring systems :
containing 1 :

G1:O,S,N

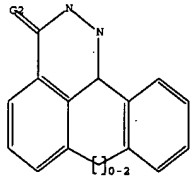
G2:O,S

G3:C,O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 19:CLASS 22:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S,N
G2 O,S
G3 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 10:38:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 41 TO ITERATE

100.0% PROCESSED 41 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 436 TO 1204
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 10:38:47 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 828 TO ITERATE

100.0% PROCESSED 828 ITERATIONS 63 ANSWERS
SEARCH TIME: 00.00.01

L3 63 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY 172.10 TOTAL SESSION 172.52
FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 10:38:51 ON 25 JAN 2007
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FILE COVERS 1907 - 25 Jan 2007 VOL 146 ISS 5
FILE LAST UPDATED: 24 Jan 2007 (20070124/ED)

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=> s l3
L4 40 L3

=> d 1-5

L4 ANSWER 1 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:829353 CAPLUS
DN 139:317471
TI Aryl and heteroaryl poly(ADP-ribose) polymerase (PARP) inhibitors, preparation, pharmaceutical compositions, and methods of therapeutic use
IN Jackson, Paul F.; Li, Jia-He; Maclin, Keith M.; Zhang, Jie
PA Guilford Pharmaceuticals Inc., USA
SO U.S., 37 pp., Cont.-in-part of U.S. Ser. No. 79,512, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 17

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6635642	B1	20031021	US 1998-145176	19980901
	US 6346536	B1	20020212	US 1997-922548	19970903
	CA 2294074	A1	19990311	CA 1998-2294074	19980902
	WO 9911649	A2	19990311	WO 1998-US18185	19980902
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9893748	A	19990322	AU 1998-93748	19980902
	EP 1012153	A1	20000628	EP 1998-946812	19980902
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
PRAI	US 1997-922520	B2	19970903		
	US 1997-922548	A2	19970903		
	US 1998-79512	B2	19980515		
	US 1998-145176	A	19980901		
	WO 1998-US18185	W	19980902		

RE.CNT 528 THERE ARE 528 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:92405 CAPLUS
DN 138:137290
TI Preparation of benzpyranoisoquinolinones and related compounds as poly(ADP-ribose)polymerase (PARP) inhibitors.
IN Li, Jia-He; Zhang, Jie; Jackson, Paul F.; Maclin, Keith M.
PA Guilford Pharmaceuticals, Inc., USA
SO U.S., 41 pp., Cont.-in-part of U.S. 6,306,889.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 17

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6514983	B1	20030204	US 1998-145181	19980901
	US 6346536	B1	20020212	US 1997-922548	19970903
	US 6306889	B1	20011023	US 1998-47502	19980325
	CA 2294133	A1	19990311	CA 1998-2294133	19980902
	WO 9911645	A1	19990311	WO 1998-US18189	19980902
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9892982	A	19990322	AU 1998-92982	19980902
	BR 9812185	A	20000718	BR 1998-12185	19980902
	EP 1019409	A1	20000719	EP 1998-945828	19980902
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	TR 200001279	T2	20001023	TR 2000-200001279	19980902
	HU 200003569	A2	20010730	HU 2000-3569	19980902
	JP 2002510332	T	20020402	JP 1999-516974	19980902
	NZ 503043	A	20021025	NZ 1998-503043	19980902
	NO 2000001001	A	20000405	NO 2000-1001	20000228
PRAI	US 1997-922548	A2	19970903		
	US 1998-47502	A2	19980325		
	US 1998-145181	A	19980901		
	WO 1998-US18189	W	19980902		

OS MARPAT 138:137290
RE.CNT 567 THERE ARE 567 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:52765 CAPLUS
DN 140:16693
TI Synthesis and biological evaluation of 2,7-dihydro-3H-dibenzo[de,h]cinnoline-3,7-dionederivatives, a novel group of anticancer agents active on a multidrug resistant cell line
AU Stefanska, Barbara; Arciemiuk, Malgorzata; Bontemps-Gracz, Maria M.; Dzieduszycka, Maria; Kupiec, Agnieszka; Martelli, Sante; Borowski, Edward
CS Department of Pharmaceutical Technology and Biochemistry, Gdansk University of Technology, Gdansk, 80-952, Pol.
SO Bioorganic & Medicinal Chemistry (2003), 11(4), 561-572
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 140:16693
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:851122 CAPLUS
DN 135:371759
TI Preparation of N-imidazolylphenyl-5,6-dihydrobenzo[h]quinazolin-4-amines and other N-containing heterocyclic amines as 5-hydroxytryptamine antagonists for treatment of CNS disorders
IN Yamada, Akira; Spears, Glen; Hayashida, Hisashi; Tomishima, Masaki; Ito, Kiyotaka; Imanishi, Masashi
PA Fujisawa Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 154 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001087845	A2	20011122	WO 2001-JP4002	20010514
	WO 2001087845	A3	20020829		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 2001056728	A5	20011126	AU 2001-56728	20010514
	US 2003176454	A1	20030918	US 2002-258582	20021101
PRAI	AU 2000-7501	A	20000515		
	AU 2000-1955	A	20001207		
	WO 2001-JP4002	W	20010514		

OS MARPAT 135:371759

L4 ANSWER 5 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:167996 CAPLUS
DN 134:207821
TI Preparation of [1]benzopyrano[4,3,2-de]phthalazine-3(2H)-ones, pharmaceutical compositions and use for treating cellular damage, such as neural or cardiovascular tissue damage
IN Li, Jia-He; Zhang, Jie
PA Guilford Pharmaceuticals Inc., USA
SO PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001016137	A1	20010308	WO 2000-US23745	20000830
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6291425	B1	20010918	US 1999-387767	19990901
	CA 2382317	A1	20010308	CA 2000-2382317	20000830
	EP 1212328	A1	20020612	EP 2000-959578	20000830
	EP 1212328	B1	20060802		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	JP 2003508400	T	20030304	JP 2001-519703	20000830
	AT 334985	T	20060815	AT 2000-959578	20000830
	US 6716828	B1	20040406	US 2001-781195	20010213
	US 2005074470	A1	20050407	US 2004-772235	20040206
	AU 2005202592	A1	20050707	AU 2005-202592	20050615
PRAI	US 1999-387767	A	19990901		
	WO 2000-US23745	W	20000830		
	US 2001-781195	A3	20010213		

OS MARPAT 134:207821
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 6-10

L4 ANSWER 6 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:184260 CAPLUS
DN 130:209323
TI Preparation of PARP inhibitors
IN Jackson, Paul F.; Li, Jia-He; Maclin, Keith M.; Zhang, Jie
PA Guilford Pharmaceuticals Inc., USA
SO PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 17

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9911649	A2	19990311	WO 1998-US18185	19980902
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6346536	B1	20020212	US 1997-922548	19970903
	US 6635642	B1	20031021	US 1998-145176	19980901
	CA 2294074	A1	19990311	CA 1998-2294074	19980902
	AU 9893748	A	19990322	AU 1998-93748	19980902
	EP 1012153	A1	20000628	EP 1998-946812	19980902
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
PRAI	US 1997-922520	A	19970903		
	US 1997-922548	A	19970903		
	US 1998-79512	A	19980515		
	US 1998-145176	A	19980901		
	WO 1998-US18185	W	19980902		

L4 ANSWER 7 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:184256 CAPLUS
DN 130:209714
TI Tetracyclic heteroaromatic compounds as poly(ADP-ribose) polymerase (PARP) inhibitors for treating neural or cardiovascular tissue damage
IN Li, Jia-He; Zhang, Jie; Jackson, Paul F.; Maclin, Keith M.
PA Guilford Pharmaceuticals Inc., USA
SO PCT Int. Appl., 122 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 17

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9911645	A1	19990311	WO 1998-US18189	19980902
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6346536	B1	20020212	US 1997-922548	19970903
	US 6306889	B1	20011023	US 1998-47502	19980325
	US 6514983	B1	20030204	US 1998-145181	19980901

	CA 2294133	A1	19990311	CA 1998-2294133	19980902
	AU 9892982	A	19990322	AU 1998-92982	19980902
	BR 9812185	A	20000718	BR 1998-12185	19980902
	EP 1019409	A1	20000719	EP 1998-945828	19980902
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	HU 200003569	A2	20010730	HU 2000-3569	19980902
	JP 2002510332	T	20020402	JP 1999-516974	19980902
	NZ 503043	A	20021025	NZ 1998-503043	19980902
	NO 2000001001	A	20000405	NO 2000-1001	20000228
PRAI	US 1997-922548	A	19970903		
	US 1998-47502	A	19980325		
	US 1998-145181	A	19980901		
	WO 1998-US18189	W	19980902		

OS MARPAT 130:209714
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1984:139054 CAPLUS
DN 100:139054
TI 3-Aryl- and 3-(aryloxy)phthalic acids in the synthesis of fluorenones and xanthones
AU Oleinik, A. F.; Adamskaya, E. V.
CS Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, 119021, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1983), (11), 1537-9
CODEN: KGSSAQ; ISSN: 0453-8234
DT Journal
LA Russian
OS CASREACT 100:139054

L4 ANSWER 9 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1978:509328 CAPLUS
DN 89:109328
TI Structure and reactions of N,N'-dialkylhydrazides of anthraquinone-1-carboxylic acid
AU Mednis, J.
CS Rizh. Politekh. Inst., Riga, USSR
SO Tezisy Dokl. - Resp. Konf. Molodykh Uch.-Khim., 2nd (1977), Volume 1, 3-4 Publisher: Akad. Nauk Est. SSR, Inst. Khim., Tallinn, USSR.
CODEN: 38RMAG
DT Conference
LA Russian

L4 ANSWER 10 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1976:42754 CAPLUS
DN 84:42754
TI Electron absorption spectra and structure of pyridazonanthrone and its amino derivatives
AU Zaitsev, B. E.; Mikhailova, T. A.; Fain, V. Ya.
CS USSR
SO Zhurnal Fizicheskoi Khimii (1975), 49(10), 2552-5
CODEN: ZFKHA9; ISSN: 0044-4537
DT Journal
LA Russian

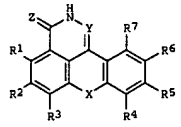
=> d ibib abs hitstr 7-40

L4 ANSWER 7 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:184256 CAPLUS
DOCUMENT NUMBER: 130:209714
TITLE: Tetracyclic heteroaromatic compounds as poly(ADP-ribose) polymerase (PARP) inhibitors for treating neural or cardiovascular tissue damage
INVENTOR(S): Li, Jia-He; Zhang, Jie; Jackson, Paul F.; Maclin, Keith M.
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 122 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9911645	A1	19990311	WO 1998-US18189	19980902
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6346536	B1	20020212	US 1997-922548	19970903
US 6306889	B1	20011023	US 1998-47502	19980325
US 6514983	B1	20030204	US 1998-145181	19980901
CA 2294133	A1	19990311	CA 1998-2294133	19980902
AU 9892982	A	19990322	AU 1998-92982	19980902
BR 9812185	A	20000718	BR 1998-12185	19980902
EP 1019409	A1	20000719	EP 1998-945828	19980902
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
HU 200003569	A2	20010730	HU 2000-3569	19980902
JP 2002510332	T	20020402	JP 1999-516974	19980902
NZ 503043	A	20021025	NZ 1998-503043	19980902
NO 2000001001	A	20000405	NO 2000-1001	20000228

PRIORITY APPLN. INFO.: US 1997-922548 A 19970903
US 1998-47502 A 19980325
US 1998-145181 A 19980901
WO 1998-US18189 W 19980902

OTHER SOURCE(S): MARPAT 130:209714
GI

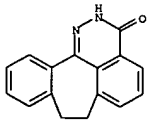


I

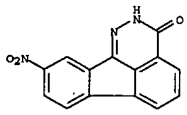
AB Title compds. I [Y = alkylhalo, alkyl-COG, COG, direct bond, CO, O, NR11, CR8; G = NR11R16, OR9, SR9, R10; Z = O, S, NR11; X = NR16, O, S, CR12R13, CO, bond, -CR12CR13, CR12R13CR14R15; R1-R8, R10, R12-R15 = H, halo, alkylhalo, OH, C1-C9 alkyl, C2-C9 alkenyl group, C3-C8 cycloalkyl, C5-C7 cycloalkenyl, aryl, amino, alkylamino, NO2, NO, CO2H, aralkyl; R9 = H, OH, C1-C9 alkyl, C2-C9 alkenyl, C3-C8 cycloalkyl, C5-C7 cycloalkenyl, aryl, NH2, alkylamino, CO2H, aralkyl; R11, R16 = H, halo, alkylhalo, OH, C1-C9 alkyl, C2-C9 alkenyl group, C3-C8 cycloalkyl, C5-C7 cycloalkenyl, aryl, NH2, alkylamino, CO2H, or aralkyl] were prepared for use as PARP inhibitors for treating neural or cardiovascular tissue damage. Thus, I [X, Z = O, Y = NH, R1-R7 = H, the dotted bond is a single bond] was prepared from 9-xanthenecarboxamide by reduction to the amine, conversion to isocyanate, and cyclization and had a PARP-inhibiting IC50 of 0.20μM.

IT 35157-46-1P 36993-60-9P 36993-62-1P
36999-81-2P, Indeno[1,2,3-de]phthalazin-3(2H)-one
220938-30-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzopyranoisoquinolinones and benzopyranophthalazinones as poly(ADP-ribose) polymerase inhibitors)

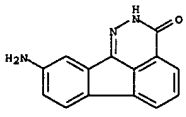
RN 35157-46-1 CAPLUS
CN Benzo[6,7]cyclohepta[1,2,3-de]phthalazin-3(2H)-one,7,8-dihydro- (9CI) (CA INDEX NAME)



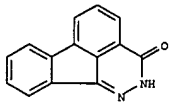
RN 36993-60-9 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one,9-nitro- (9CI) (CA INDEX NAME)



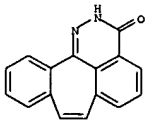
RN 36993-62-1 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one,9-amino- (9CI) (CA INDEX NAME)



RN 36999-81-2 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one(7CI, 8CI, 9CI) (CA INDEX NAME)

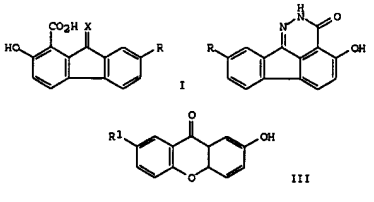


RN 220938-30-7 CAPLUS
CN Benzo[6,7]cyclohepta[1,2,3-de]phthalazin-3(2H)-one(9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

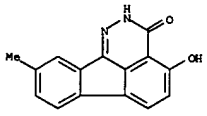
L4 ANSWER 8 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:139054 CAPLUS
DOCUMENT NUMBER: 100:139054
TITLE: 3-Aryl- and 3-(aryloxy)phthalic acids in the synthesis of fluorenones and xanthones
AUTHOR(S): Oleinik, A. F.; Adamskaya, E. V.
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, 119021, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1983), (11), 1537-9
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 100:139054
GI



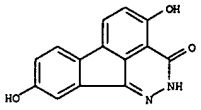
I II III

AB Fluorenones I (R = Me, OH, X = O), prepared in 70 and 66% from the corresponding phthalic anhydride, were treated with N2H4.H2O to give 76% I

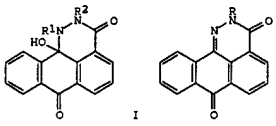
(X = NNH2), which underwent intramol. cyclocondensation by heating in vacuo at 180-200° to give 42% II. Xanthenones III (R1 = Me, H) were also obtained from the corresponding 3-phenoxyphthalic anhydride.
IT 89450-85-1P 89450-86-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 89450-85-1 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one,4-hydroxy-9-methyl- (9CI) (CA INDEX NAME)



RN 89450-86-2 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one,4,9-dihydroxy- (9CI) (CA INDEX NAME)



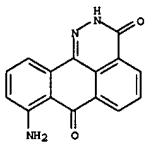
L4 ANSWER 9 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:509328 CAPLUS
DOCUMENT NUMBER: 89:109328
TITLE: Structure and reactions of N,N'-dialkylhydrazides of anthraquinone-1-carboxylic acid
AUTHOR(S): Mednis, J.
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR
SOURCE: Tezisy Dokl. - Resp. Konf. Molodykh Uch.-Khim., 2nd (1977), Volume 1, 3-4. Akad. Nauk Est. SSR, Inst. Khim.: Tallinn, USSR.
CODEN: 38RMAG
DOCUMENT TYPE: Conference
LANGUAGE: Russian
GI



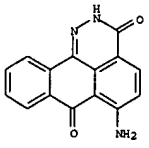
I

II

RN 57981-26-7 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-amino- (7CI, 9CI) (CA INDEX NAME)

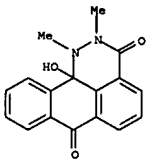


RN 57981-27-8 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-amino- (7CI, 9CI) (CA INDEX NAME)

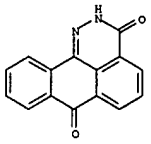


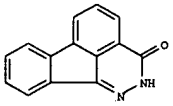
L4 ANSWER 11 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:4857 CAPLUS
DOCUMENT NUMBER: 84:4857
TITLE: Polycyclic fused amidines. II. Synthesis of dihydroimidazo-fused systems by use of aminoethylammonium p-toluenesulfonate
AUTHOR(S): Cookson, Ronald F.; Rodway, Ronald E.
CORPORATE SOURCE: Nicholas Res. Lab., Slough, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1975), (19), 1854-7
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 84:4857
GI For diagram(s), see printed CA Issue.
AB Heating NH2(CH2)2N+H3 p-MeC6H4SO3- (I) with phthalazinones, quinolones, and isoquinolines at 200-50° gave the corresponding dihydroimidazo compds. E.g., I with phthalazin-2-one gave 20% II. The imidazoquinoxalines III (R = H, Ph) were prepared by cycloaddn. of 2-chloroquinoxaline and its 3-phenyl derivative with NH2CH2CH(OMe)2.
IT 36999-81-2 58106-74-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction with aminoethylammonium toluenesulfonate)
RN 36999-81-2 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one(7CI, 8CI, 9CI) (CA INDEX NAME)

AB Treatment of I (R1 = R2 = Me, R1R2 = o-H2CC6H4CH2) with SOCl2 or HCl under mild conditions gave II (R = Me, o-C6H4CHO).
IT 53453-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thionyl chloride and hydrochloric acid)
RN 53453-78-4 CAPLUS
CN 1H-Dibenzo[de,h]cinnoline-3,7(2H,11bH)-dione,11b-hydroxy-1,2-dimethyl- (9CI) (CA INDEX NAME)

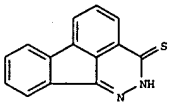


L4 ANSWER 10 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:42754 CAPLUS
DOCUMENT NUMBER: 84:42754
TITLE: Electron absorption spectra and structure of pyridazonanthrone and its amino derivatives
AUTHOR(S): Zaitsev, B. E.; Mikhailova, T. A.; Fain, V. Ya.
CORPORATE SOURCE: USSR
SOURCE: Zhurnal Fizicheskoi Khimii (1975), 49(10), 2552-5
CODEN: ZFKHA9; ISSN: 0044-4537
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB The long-wavelength band in the electronic absorption spectrum of I was assigned to an Sπ* transition involving charge transfer from the pyridazone ring to the anthrone ring. The analogous band for the 4-amino, 5-amino, and 5-amino-N-phenyl derivs. was assigned to an S2pz* transition involving charge transfer from the amino N to the ring π system. Atomic charge densities were calculated
IT 731-37-3 57981-26-7 57981-27-8
RL: PRP (Properties)
(uv-visible spectrum of, solvent effect on)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)

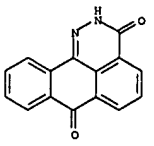




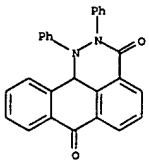
RN 58106-74-4 CAPLUS
CN Indeno[1,2,3-de]phthalazine-3(2H)-thione(7CI, 9CI) (CA INDEX NAME)



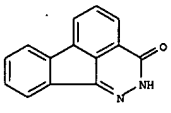
L4 ANSWER 12 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:3986 CAPLUS
DOCUMENT NUMBER: 84:3986
TITLE: Infrared absorption spectra and structure of oxazon- and pyridazonanthrone and their derivatives
AUTHOR(S): Zaitsev, B. E.; Mikhailova, T. A.; Fain, V. Ya.
CORPORATE SOURCE: Nauchno-Issled. Inst. Org. Poluprod. Krasitelei, Moscow, USSR
SOURCE: Zhurnal Fizicheskoi Khimii (1975), 49(9), 2194-9
CODEN: ZFKHA9; ISSN: 0044-4537
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB The ir data for I (X = O, NH, NPh, NC6H4Br-p, NC6H4NO2-p; R, R1 = H, NH2) and related compds. indicated that the dioxo forms predominate. In I (R or R1 = NH2), H bonding exists between the NH2 group and the carbonyl O; the stability of the H bond is greater when R = NH2.
IT 731-37-3 57449-83-9
RL: PRP (Properties)
(ir spectrum of)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



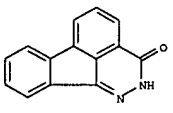
RN 57449-83-9 CAPLUS
CN 1H-Dibenzo[de,h]cinnoline-3,7(2H,11bH)-dione,1,2-diphenyl- (9CI) (CA INDEX NAME)



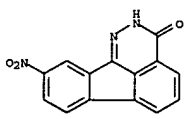
L4 ANSWER 13 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:427978 CAPLUS
DOCUMENT NUMBER: 83:27978
TITLE: 1-Phenylnaphthalenes. IX. Reactions of 7-bromo-1-p-bromophenylnaphthalene-2,3-dicarboxylic acid anhydride and ketoesters with Grignard reagents and hydrazine derivatives
AUTHOR(S): Baddar, F. G.; Sherif, Sayed; Shenouda, Ibrahim G.
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
SOURCE: Egyptian Journal of Chemistry (1974), Volume Date 1973, (Spec. Issue), 145-57
CODEN: EGJCA3; ISSN: 0449-2285
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The Grignard reaction of the anhydride (I) gave ten naphthofuranones (II; R = Me, Et, PhCH2, Ph, 1-naphthyl, substituted phenyl). I with N2H4 and PhNHNH2 gave the phthalazine (III) and the resp. N-anilino imide.
IT 36999-81-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36999-81-2 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one(7CI, 8CI, 9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:520557 CAPLUS
DOCUMENT NUMBER: 81:120557
TITLE: Effect of the rigid conformation of thecarbonyl group on ring-chain isomerism of anthraquinone-1-carboxylic acid derivatives
AUTHOR(S): Valters, R.; Mednis, J.
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1974), 10(6), 1248-52
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian

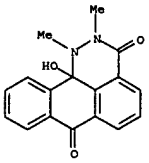


L4 ANSWER 16 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:461927 CAPLUS
DOCUMENT NUMBER: 77:61927
TITLE: Fluorenone-1-carboxylic acid and aza analogs of fluoranthene
AUTHOR(S): Zinchenko, V. M.; Burmistrov, S. I.
CORPORATE SOURCE: Dnepropetr. Khim.-Tekhnol. Inst., Dnepropetrovsk, USSR
SOURCE: Khimicheskaya Tekhnologiya (Kharkov) (1971), No. 21, 105-9
CODEN: KTRMAQ; ISSN: 0368-699X
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Oxidation of fluoranthene by K2Cr2O7 in concentrated H2SO4 for 1 hr gave 28-30% title compound (I), which was reduced by Na2S2O4 to give 93-5% of the corresponding hydroxy acid. Nitration of fluorene-1-carboxylic acid by HNO3-H2SO4 gave the 7-NO2 derivative (II), which was reduced by Na2S to the 7-amino derivative (III). Treatment of I with PhNHNH2 gave the phenylhydrazone which was cyclized by azeotropic distillation with xylene for 3-4 hr to give 3-phenyl-4-oxo-2,3-diazadihydrofluoranthene(IV). Similarly, 4-hydroxy-2,3-diazafluoranthenewas obtained from I, 12-nitro-4-oxo-2,3-diazadihydrofluroanthenefrom II, and 12-amino-4-oxo-2,3-diazafluoranthenefrom III.
IT 36993-60-9P 36993-61-0P 36993-62-1P
36999-81-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36993-60-9 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one,9-nitro- (9CI) (CA INDEX NAME)

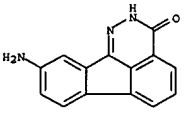


RN 36993-61-0 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one,9-amino-, monohydrochloride (9CI) (CA INDEX NAME)

GI For diagram(s), see printed CA Issue.
AB Anthraquinonecarboxamides (I; R = H, Me, Et, Me2CH, Ph, NMe2) were obtained in 22-63% yields by amination of anthraquinone-1-carbonyl chloride (II) with RNH2. Treatment of II with MeNHNH2 in Et3N gave dibenzocinnoline (III).
IT 53453-78-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53453-78-4 CAPLUS
CN 1H-Dibenzo[de,h]cinnoline-3,7(2H,11bH)-dione,11b-hydroxy-1,2-dimethyl-(9CI) (CA INDEX NAME)

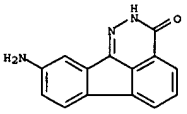


L4 ANSWER 15 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:437417 CAPLUS
DOCUMENT NUMBER: 81:37417
TITLE: 1-Phenylnaphthalenes. IX. Reactions of 7-bromo-1-p-bromophenylnaphthalene-2,3-dicarboxylic anhydride and certain keto esters with Grignard reagents and hydrazine derivatives
AUTHOR(S): Baddar, F. G.; Sherif, Sayed; Shenouda, Ibrahim G.
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
SOURCE: Egyptian Journal of Chemistry (1973), (Special), 145-57
CODEN: EGJCA3; ISSN: 0449-2285
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Reaction of the title anhydride (I) with RMgX (R = Me, Et, PhCH2, Ph, p-ClC6H4, o-, m-, p-MeC6H4, p-MeOC6H4, 1-naphthyl) gave 66-98% lactones (II). Treating I with AlCl3 at <10° gave cyclic ketone (III; R = OH). Conversion of III (R = OH) to III (R = Cl) followed by reaction with a hydrocarbon, e.g., C6H6, PhMe, or PhCl, gave 20-94% III (R = Ph, p-MeC6H4, p-ClC6H4). Treatment of III (R = OMe) with MeMgI or p-ClC6H4MgBr gave the alc. (IV; R1 = Me, p-ClC6H4) in 82 and 43% yield, resp. Reaction of I with N2H4 and PhNHNH2 gave the cyclic compds. (V and VI) in 67 and 83% yield, resp.
IT 36999-81-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36999-81-2 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one(7CI, 8CI, 9CI) (CA INDEX NAME)

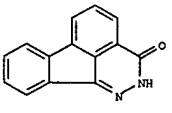


● HCl

RN 36993-62-1 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one,9-amino- (9CI) (CA INDEX NAME)

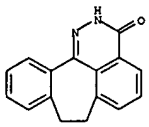


RN 36999-81-2 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one(7CI, 8CI, 9CI) (CA INDEX NAME)

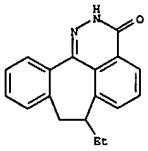


L4 ANSWER 17 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:85774 CAPLUS
DOCUMENT NUMBER: 76:85774
TITLE: Synthesis of new heterocyclic systems. Derivatives of 5-H-dibenzo[a,d]cycloheptene
AUTHOR(S): Mavoungou-Gomes, Louis
CORPORATE SOURCE: Fac. Libre Sci., Angers, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1972), 274(1), 73-6
CODEN: CHDCAQ; ISSN: 0567-6541
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB 3-Chloro-7,8-dihydro-6,7-benzocyclohepta-[1,2,3-de]phthalazine (I) and II are prepared from III. III reacts with HONH2 and hydrazine to give IV and V. V is treated with POCl3 to give I which is converted to VI and VII. II is formed by the reaction of VII with formic acid, and VII is treated with HNO2 to give the tetrazolo phthalazine (VIII).
IT 35157-46-1P 35157-48-3P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 35157-46-1 CAPLUS
CN Benzo[6,7]cyclohepta[1,2,3-de]phthalazin-3(2H)-one,7,8-dihydro- (9CI) (CA INDEX NAME)



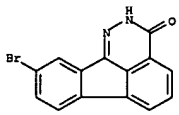
RN 35157-48-3 CAPLUS
CN Benzo[6,7]cyclohepta[1,2,3-de]phthalazin-3(2H)-one,7-ethyl-7,8-dihydro- (9CI) (CA INDEX NAME)



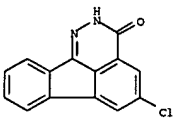
L4 ANSWER 18 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:14566 CAPLUS
DOCUMENT NUMBER: 76:14566
TITLE: Indeno[1,2,3-de]phthalazines
INVENTOR(S): Rodway, Ronald E.; Simmonds, Robin G.
PATENT ASSIGNEE(S): Aspro-Nicholas Ltd.
SOURCE: Ger. Offen., 30 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2111910	A	19711007	DE 1971-2111910	19710312
ZA 7101512	A	19711229	ZA 1971-1512	19700308
US 3803146	A	19740409	US 1971-123061	19710310
BE 764203	A1	19710913	BE 1971-100863	19710312
FR 2085706	A1	19711231	FR 1971-8641	19710312
FR 2085706	A5	19711231		
CH 525218	A	19720715	CH 1971-525218	19710312
PRIORITY APPLN. INFO.:			GB 1970-12424 A	19700314

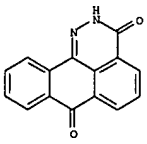
GI For diagram(s), see printed CA Issue.
AB The title compds. [I; where R = 4-(β-hydroxyethyl)-1-piperazinyl, 4-ethoxycarbonyl-1-piperazinyl, Me2N, HOCH2CH2NH, 3-morpholinopropylamino, 1-piperazinyl, 4-allyl-1-piperazinyl, HO(CH2)3NH, 4-acetyl-1-piperazinyl, or cyclopropylamino; R1 = H or Cl; R2 = H or Br] and their salts of antiinflammatory and antirheumatic activities were prepared by condensation of the 3-chloro derivative (I, R = Cl) (II) with HR optionally followed by transalkylation. Thus, 8.8 g II and 11 g 4-(β-hydroxyethyl)piperazine in dioxane was refluxed 3 hr to give 8 g I [R = 4-(β-hydroxyethyl)-1-piperazinyl, R1 = R2 = H]. Similarly prepared were 11 other I.
IT 34642-24-5P 34642-29-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 34642-24-5 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one,9-bromo- (9CI) (CA INDEX NAME)



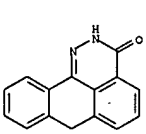
RN 34642-29-0 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one,5-chloro- (9CI) (CA INDEX NAME)



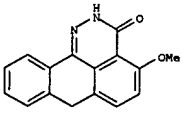
L4 ANSWER 19 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:111797 CAPLUS
DOCUMENT NUMBER: 74:111797
TITLE: Anthracenes from benzyl furans
AUTHOR(S): Mavoungou-Gomes, Louis
CORPORATE SOURCE: Fac. Libre Sci., Angers, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1971), 272(7), 687-90
CODEN: CHDCAQ; ISSN: 0567-6541
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB The anthrone I was prepared by treating the adduct from 2-benzylfuran and MeO2CC.tplbond.CCO2Me with BF3, methylating the phenolic OH of 4,2,3-PhCH2(MeO2C)2-C6H2OH, saponification and dehydration to the anhydride, and cyclization with AlCl3. I and II were lactonized with Ac2O, converted to dibenzo[c,d,g]indoles with amines, or converted to 7H-dibenzo[d,e,h]cinnolines with hydrazines. The dibenzocinnolines showed no tautomerism. Cr2O3 oxidation of II gave 1-carboxyanthraquinone. 2-Oxo-4,5-dihydro-2H-anthra[9,1-bc]-furan was similarly prepared from the adduct of 2-benzylfuran with maleic anhydride.
IT 731-37-3P 31272-82-9P 31272-83-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



RN 31272-82-9 CAPLUS
CN 3H-Dibenzo[de,h]cinnolin-3-one,2,7-dihydro- (8CI) (CA INDEX NAME)



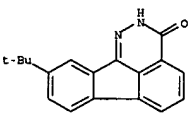
RN 31272-83-0 CAPLUS
CN 3H-Dibenzo[de,h]cinnolin-3-one,2,7-dihydro-4-methoxy- (8CI) (CA INDEX NAME)



L4 ANSWER 20 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1969:115926 CAPLUS
DOCUMENT NUMBER: 70:115926
TITLE: Ultraviolet stabilizers for plastics
INVENTOR(S): Hofer, Kurt; Schilli, Alfred
PATENT ASSIGNEE(S): Sandoz Ltd.
SOURCE: Patentschrift (Switz.), 6 pp.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 463778		19681129	CH 1965-17531	19651012

GI For diagram(s), see printed CA Issue.
AB Compds. prepared from pyromellitic acid or the anhydride with hydrazine or its derivs. were used to stabilize poly(vinyl chloride), polystyrene, or polyolefins against heat and uv light. Thus, a mixture of 7-tert-butyl-9-oxofluorene-1-carboxylicacid 28, MeOH 60, and hydrazine hydrate 15 parts was refluxed for 6 hrs., the mixture filtered, the residue washed with water, dried, and recrystd. from dioxane to give 12-tert-butyl-4-hydroxy-2,3-diazafluoranthene(I), m. 275-8°. Similarly prepared were 5,12-di-tert-butyl-4-hydroxy-2,3-diazafluoranthene and 12-hexyl-4-hydroxy-2,3-diazafluoranthene. A mixture of 100 parts polystyrene and 0.1 part I was pressed into a 1 mm. thick disk at 180° and 30 tons pressure. The clear disks absorbed uv light in the region of 290-370 mμ. and after 160 hrs. in the Xenotest apparatus showed a uv absorption loss of only 5%. Other compds. similarly used were II (R and m.p. given): 3-ClC6H4, 160-1°; C2H4OH, 202-3°; CH2CHOHMe, 88-92°; CH2CHOHPh, 110-17°; C2H4O2CEt, 118-20°; C2H4O2CPr, 71-4°; and C2H4OCC7H15, 48-52°. Other compds. used were III (R given): H; Bu; Ph; Me. Also used were 1,4-dioxo-1,2,3,4-tetrahydrophthalazine-6-carboxylate, 7,7'-carbonylbis(1,4-dioxo-1,2,3,4-tetrahydrophthalazine), and 2-methyl-4-(p-tolyl)phthalazin-1(2H)-one, m. 149-50°. Most of these compds. have a uv absorption maximum varying from 307 to 315 mμ, from 290 to 375 mμ., or from 325 to 335 mμ. Also stabilized was polyethylene.
IT 19117-42-1
RL: USES (Uses)
(as stabilizer for chloroethylene polymers)
RN 19117-42-1 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3-ol,9-tert-butyl- (8CI) (CA INDEX NAME)



L4 ANSWER 21 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1968:487767 CAPLUS
DOCUMENT NUMBER: 69:87767
TITLE: Improving the light stability of organic compositions, especially polyolefins, polystyrene, and poly(vinyl chlorides)
INVENTOR(S): Hofer, Kurt; Schilli, Alfred
PATENT ASSIGNEE(S): Sandoz Ltd.
SOURCE: Fr., 7 pp.
CODEN: FRXXAK
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1502917		19671124	FR 1966-79501	19661011
DE 1593443			DE	
GB 1175845			GB	
US 3497512		19700224	US	19661010
PRIORITY APPLN. INFO.:			CH	19651012

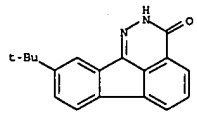
GI For diagram(s), see printed CA Issue.
AB Compds. such as 12-tert-butyl-4-hydroxy-2,3-diazafluoranthene, 6,7-diaza-5,8-dioxo-5,6,7,8-tetrahydroquinoline, and 2,3,6,7-tetraaza-1,4,5,8-tetraoxo-1,2,3,4,5,6,7,8-octahydroanthracene(I) are used as light absorbers (290-400 mμ) for the title polymers, cellulose acetate, and

oils. The light-absorbing compds. are prepared by known reactions between aryldicarboxylic acids and hydrazines. Thus, polypropylene was mixed with 0.25% I for 1 min. at 150° and then molded at 150°. The material absorbed strongly at 370 mμ, and the absorption was only slightly diminished after 700 hrs. of irradiation in a Xenotest apparatus

IT 19117-42-1
RL: USES (Uses)
(as ultraviolet stabilizer for oils and polymers)

RN 19117-42-1 CAPLUS

CN Indeno[1,2,3-de]phthalazin-3-ol,9-tert-butyl- (8CI) (CA INDEX NAME)



L4 ANSWER 22 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:19290 CAPLUS

DOCUMENT NUMBER: 64:19290

ORIGINAL REFERENCE NO.: 64:3526h,3527a-h

TITLE: Addition of Grignard reagents to pyridazines. IV. tert-Butylmagnesium chloride and 3-methoxy-6-phenylpyridazine

AUTHOR(S): Crossland, Ingolf; Rasmussen, Leif Kjaergaard

CORPORATE SOURCE: Tech. Univ., Copenhagen

SOURCE: Acta Chemica Scandinavica (1965), 19(7), 1652-60
CODEN: ACHSE7; ISSN: 0904-213X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB cf. CA 62, 5274d. To a stirred suspension of 18.6 g. 3-methoxy-6-phenylpyridazine (I) (an improved procedure of Gabriel and Colman (Ber. 32, 395(1899)) in 200 ml. ether was added in 5 min. a solution of tert-BuMgCl (Puntambeker and Zoellner, Organic Synthesis Collective Volume I, 524(1941)) (155 ml.). After stirring the brownish yellow reaction mixture 5 min. and decomposition of the complex with 40 ml. MeOH in 100 ml. ether, the precipitate was filtered off and washed with 200 ml. ether. The combined yellow filtrates were concd. in vacuo and gave 24 g. yellow oil containing 4-tert-butyl-3-methoxy-6-phenyl-4,5-dihydropyridazine(II) and 5-tert-butyl-3-methoxy-6-phenyl-4,5-dihydropyridazine(III). This oil was dissolved in HCl (150 ml. concentrated HCl and 150 g. ice). A small piece of solid CO2 was added to remove O and the solution kept 48 hrs. at room temperature The precipitate was filtered off, washed with water and dried in vacuo to give a light tan product which was crystallized to give 5.5 g. 4-tert-butyl-1,4,5,6-tetrahydro-6-oxo-3-phenylpyridazine (IV), m. 192-3°(alc.). The combined filtrates were cooled to -80° to give 14.4 g. Me α-tert-butyl-β-benzoylpropionate (V), m. 38-9° (petr. ether). V was saponified by NaOH-EtOH to give α-tert-butyl-β-benzoylpropionic acid (VI), m. 130-1° (ligroine). VI (6 g.) was heated to boiling with 10 ml. Ac2O and immediately poured into 70 ml. water. After stirring 1 hr. the separated crystals were washed with water and air-dried to give 5.3 g. α-tert-butyl-γ-phenyl Δ(β,γ)-butenolide, m. 69-70° (ligroine). VI was also prepared from tert-butylsuccinic anhydride and benzene by Friedel-Crafts synthesis (cf. Somerville and Allen, Organic Synthesis Collective Volume II, 81(1943)). IV (0.5 g.) was refluxed 3 hrs. with 2 ml. concentrated HBr, the mixture was cooled, the precipitate filtered off, dissolved in dilute NaOH, decolorized with Norite and acidified with HCl to give β-tert-butyl-β-benzoyl-propionic acid, m. 124-5° (aqueous alc.). The latter (6 g.) was refluxed with 10 ml. Ac2O 1 hr. and the product distilled in vacuo to give 3.7 g. β-tert-butyl-γ-phenyl Δ(α,β)-butenolide, b0.6 150-2°; m. 101-2° (ligroine). V (39.6 g.) was refluxed 48 hrs. with 10 g. 80% N2H4.H2O in 60 ml. 4N HCl. After cooling for 5 hrs., the crystals were filtered off, washed with aqueous EtOH and dried to yield 34.7 g. 5-tert-butyl-1,4,5,6-tetrahydro-6-oxo-3-phenylpyridazine,m. 161-2° (alc.). To the latter (34.7 g.) in 50 ml. AcOH was added with stirring 7.7 ml. Br keeping the temperature at 90 to 100°. After evolution of HBr, water was added and the crystals filtered off, washed with water and aqueous EtOH and dried to give 36 g. 5-tert-butyl-1,4,5,6-tetrahydro-4-bromo-6-oxo-3-phenylpyridazine(VII), m. with decomposition (EtOH). VII (36 g.) was dissolved in a solution of NaOMe (2.8 g. Na in 100 ml. MeOH) at reflux, then cooled to 15°, diluted with 100 ml. H2O, the precipitate filtered off, washed with aqueous MeOH and dried to give 30.3 g.

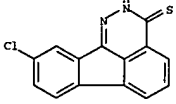
5-tert-butyl-1,6-dihydro-6-oxo-3-phenylpyridazine(VIII), m. 180-3° (alc.). VIII (30.3 g.) was refluxed in 169 ml. POCl3 for 7 hrs., poured into ice, neutralized with NH3 and extracted with CHCl3. The organic layer was charcoaled, dried over MgSO4 and CHCl3 removed to give 18.2 g. 4-butyl-3-chloro-6-phenyl-pyridazine,m. 74-5° (petr. ether). This (18.2 g.) was refluxed 5 hrs. in NaOMe (4 g. Na in 100 ml. MeOH), H2O was added and the product extracted with CHCl3, the organic phase charcoaled, dried and CHCl3 removed in vacuo to give 17.6 g. 4-tert-butyl-3-me-thoxy-6-phenylpyridazine (IX), m. 73-5° (petr. ether). To an ethereal solution of II and III (prepared from 18.6 g. I) was added cold HCl (50 ml. concentrated HCl and ice in excess) and well stirred. The aqueous phase was cooled by adding more ice and then 6.5 ml. Br was added and the mixture shaken and then extracted with CHCl3. The combined CHCl3 layers were shaken vigorously with 100 ml. cold aqueous NH3 (28%) and ice, dried over MgSO4 and CHCl3 removed in vacuo to give 17.6 g. 4-tert-butyl-5-bromo-3-methoxy-6-phenyl-4,5-dihydropyridazine (X), m. 134-6° (decomposition) (ligroine) (with fast heating decompose at 150°). X (4.2 g.) was dissolved in 42 ml. EtOH at reflux temperature, kept at room temperature for 4 days and the precipitate filtered off to give 1.2 g. salt, crystallized from EtOH. This was heated with hot CHCl3 and the precipitate (1.2 g.) dissolved in CHCl3 (10 ml. and 10 ml. water) by stirring for 2 hrs. The organic layer was evaporated in vacuo to give 0.4 g.

IX. X (14.8 g.) refluxed for 24 hrs. with NaOMe (2.5 g. Na in 100 ml. MeOH), diluted with water and extracted with CHCl3, dried with MgSO4 and CHCl3 removed gave 8.6 g. IX. X (815 mg.) was heated to 130° (bath temperature). The bath was removed when the reaction became too vigorous. MeBr (223 mg.) was collected at -80°. The product was finally heated to 142°. The residue (573 mg.) gave 412 mg. VIII. X (5 g.) was dissolved in 20 ml. concentrated HCl and allowed to stand 6 days at room temperature H2O was added and the crystals filtered off to give 3.5 g. VII. To the ethanolic mother liquor (100 ml.) from the recrystn. of X was added NaOMe (from 2.3 g. Na) and the dark solution refluxed 16 hrs. Addition of H2O and extraction with CHCl3 gave 6.8 g. yellow oil, b0.5-0.7 150-60°, consisting mainly of IX and 5-tert-butyl-3-methoxy-6-phenylpyridazine (XI). Pure IXa and XI, m. 69-70° (petroleum ether) were obtained by chromatography on silica gel, eluted with C6H6-ether.

IT 859040-00-9P, Indeno[1,2,3-de]phthalazine-3(2H)-thione,9-chloro-
RL: PREP (Preparation)
(preparation of)

RN 859040-00-9 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



L4 ANSWER 23 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1965:439103 CAPLUS

DOCUMENT NUMBER: 63:39103

ORIGINAL REFERENCE NO.: 63:7006b-d

TITLE: 1,9-Substituted derivatives fluorene. II. 2-Methyl(phenyl)2,3H-pyridazino[4,5,6-m,l]fluoren-3-one and -thione

AUTHOR(S): Dokunikhin, N. S.; Mikhalenko, S. A.

SOURCE: Zhurnal Organicheskoi Khimii (1965), 1(5), 944-6
CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

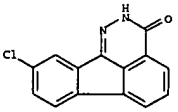
LANGUAGE: Russian

AB cf. CA 59, 10037b. 1-Fluorenonecarboxylic acid heated in AcOH with MeNHNH2.HCl and NaOAc 4 hrs. gave 2-methyl-2,3H-pyridazino[4,5,6-m,l]fluoren-3-one (I) 59% m. 154-5°. Similarly were prepared: 2-methyl-9-chloro analog, 75%, m. 233-4.1°; 2,9-dimethyl analog, 76.5%, m. 155.7-57°. Heating 7-chloro-fluorenone-1-carboxylicacid with N2H4 in MeOH 2 hrs. gave 9-chloro-2,3H-pyridazino[4,5,6-m,l]fluoren-3one, m. 345-5.5°; similarly was prepared the 9-methyl analog, m. 290-2°. 2,3H-Pyridazino[4,5,6-m,l]-3-fluorenoneheated with Me2SO4 in C6H3Cl3 in the presence of K2CO3 gave 22.8% I; its analogs shown above were also prepared similarly. Fluorenone-1carboxylic acid heated 4 hrs. in AcOH with PhNHNH2 and NaOAc gave 94.7% 2-phenyl-2,3H-pyridazino[4,5,6-m,l]-3fluorenone, m. 223-5°. I and P2S5 heated 20 hrs. in pyridine gave 2-methyl-2,3H-pyridazino[4,5,6-m,l]-3-fluorenethione,m. 163-5°; similarly were prepared the analogs: 9-chloro-2-methyl, m. 21314.5°; 2,9-dimethyl, m. 219-20.5°; 2-phenyl, m. 264-5°.

IT 2209-50-9P, Indeno[1,2,3-de]phthalazine-3(2H)-one,9-chloro-
2209-51-0P, Indeno[1,2,3-de]phthalazine-3(2H)-one,9-methyl-
RL: PREP (Preparation)
(preparation of)

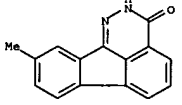
RN 2209-50-9 CAPLUS

CN Indeno[1,2,3-de]phthalazin-3(2H)-one,9-chloro- (7CI, 9CI) (CA INDEX NAME)



RN 2209-51-0 CAPLUS

CN Indeno[1,2,3-de]phthalazin-3(2H)-one,9-methyl- (7CI, 9CI) (CA INDEX NAME)



L4 ANSWER 24 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1965:58984 CAPLUS

DOCUMENT NUMBER: 62:58984

ORIGINAL REFERENCE NO.: 62:10446a

TITLE: 2 - Alkyl(aryl) - 2,3H - pyridazino[4,5,6-m,l]fluorene-3-thiones

INVENTOR(S): Dokunikhin, N. S.; Mikhalenko, S. A.

PATENT ASSIGNEE(S): Scientific-Research Institute of Organic Intermediates and Dyes

SOURCE From: Byul. Izobret. i Tovarnykh Znakov 1964(16), 12..

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

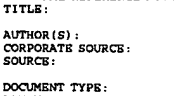
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 164604		19640819	SU	19630713
PRIORITY APPLN. INFO.:			SU	19630713

AB The title compds. were prepared by boiling 2-alkyl(aryl)-2,3H-pyridazino[4,5,6-m,l]fluoren-3-oneswith P2S5 in C5H5N.

IT 58106-74-4, Indeno[1,2,3-de]phthalazine-3(2H)-thione
(2-alkyl(or aryl) derivs.)

RN 58106-74-4 CAPLUS

CN Indeno[1,2,3-de]phthalazine-3(2H)-thione(7CI, 9CI) (CA INDEX NAME)



L4 ANSWER 25 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1965:51639 CAPLUS

DOCUMENT NUMBER: 62:51639

ORIGINAL REFERENCE NO.: 62:9129e-h

TITLE: Pyridazoanthrone and its derivatives. III. Oxazoanthrone and its connection with pyridazoanthrone

AUTHOR(S): Dokunikhin, N. S.; Fain, V. Ya.

CORPORATE SOURCE: Res. Inst. Org. Intermed. and Dyes, Rubezhnoe

SOURCE: Zhurnal Obshchei Khimii (1964), 34(11), 3769-71
CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

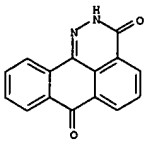
LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB cf. CA 62, 4027e. Oxazoanthrone (I) (cf. Ullmann and van der Schalk, Ann. 388, 199(1912)) heated in AcOH with N2H4 6 hrs. gave 30.1%

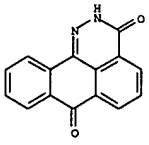
pyridazoanthrone, m. 425-6°. Similarly, PhNHNH2 gave N-phenylpyridazoanthrone (II), m. 290.3-1.0°. I heated with Br in AcOH in a sealed tube 2.5 hrs. at 150° gave after an aqueous treatment anthraquinone-1-carboxylic acid, m. 292-3°. I refluxed with 98% HNO3 gave the same acid in 88% yield. 4-Aminoanthraquinone-1-carboxylic acid refluxed 0.5 hr. with aqueous KOAc and HONH2.H2SO4, then with aqueous NH4OH, gave on acidification 78.3% 4-aminooxazoanthrone, decomposed 291°. Similarly was prepared 83.3% 5-aminooxazoanthrone, decomposed 283°. Anthraquinone-1,4-dicarboxylic acid refluxed as above with HONH2.H2SO4 gave anthra-1,9(N),10(N),4-dioxazone (III), decomposed 318-19°. Spectral data (uv) on these products were reported.

IT 731-37-3F, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione
RL: PREP (Preparation)
(preparation of)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



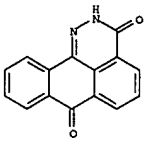
L4 ANSWER 26 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:51638 CAPLUS
DOCUMENT NUMBER: 62:51638
ORIGINAL REFERENCE NO.: 62:9129d-e
TITLE: Ion exchangers with complex-forming anchor groups. XII. Existence of ethylenediaminetriacetic acid
AUTHOR(S): Kuehn, G.; Hoyer, E.; Hering, R.
CORPORATE SOURCE: Karl-Marx-Univ., Leipzig, Germany
SOURCE: Zeitschrift fuer Chemie (1964), 4(12), 462-3
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German
AB cf. CA 60, 1142g. Me 1-aziridinylacetate (9.5 g.) and 35 g. (EtO2CCH2)2NH was heated 25 hrs. at 80° in 45 ml. alc. with a few drop alc. HCl to give 40% the Me Et (I) ester of 2-oxopiperazine-N,N'-diaceticacid, b0.001 143-5°, n20D 1.4813. Saponification of I with Ba(OH)2 gave the lactam of ethylenediaminetriacetic acid, 2-oxopiperazine-N,N'-diacetic acid (II), decomposed 214-15°. The 1:1 Cu2+ complex of II with 3 moles H2O crystallized in fine light blue needles from a solution of II and CuNO3; at 120°, 2 moles H2O were lost and the other mole was lost at 135-40°. Titration curves and stability consts. of the acid and the Ca2+, Cu2+, and Ni2+ complexes shows the inductive effect of the oxo group makes II more acid than piperazine-N,N'-diacetic acid.

IT 731-37-3F, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione
RL: PREP (Preparation)
(preparation of)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



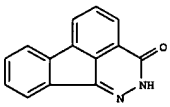
L4 ANSWER 27 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:22573 CAPLUS
DOCUMENT NUMBER: 62:22573
ORIGINAL REFERENCE NO.: 62:4027d-h,4028a
TITLE: Pyridazoanthrone and its derivatives. II. N-Arylpyridazoanthrones
AUTHOR(S): Dokunikhin, N. S.; Fain, V. Ya.
CORPORATE SOURCE: Res. Inst. Org. Intermed. and Dyes, Rubezhnoe
SOURCE: Zhurnal Obshchei Khimii (1964), 34(10), 3354-9
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. CA 55, 24699a; 61, 9493b. Refluxing anthra[9,1-cd]pyridazine-2,6-dione with the appropriate halo compound in PhNO2 in the presence of KOAc, powdered Cu, and Cu(OAc)2 10 hrs. gave 1-arylanthra[9,1-cd]pyridazine-2,6-diones (aryl group shown): 72% Ph (I), m. 287.6-89°; p-O2NC6H4, 68.7%, m. 367-8° (o-isomer, 67.3%, m. 266.7-8.3°); 2,4-(O2N)2C6H3, 84.7%, m. 314-14.8°; 1-anthraquinolyl, 78.8%, m. 338-9°; 4-methyl-1-anthraquinonyl, 78.5%, m. 367-8°; 3-benzanthronyl, 77.2%, m. 380-1°. Similarly prepared were 4',7-dinitro-1-phenylanthra[9,1-cd]pyridazine-2,6-dione,21.3%, m. 372-4°; and its ,2'7-dinitro analog, 17%, m. 285-6.5°. Refluxing 4-aminoanthraquinone-1-carboxylicacid with PhNHNH2 in 50% AcOH and NaOAc 0.5 hr. gave 60% yellow 5-amino-1-phenyl-anthra[9,1-cd]pyridazine-2,6-dione, m. 338.6-9.8°; this was formed similarly in 78.8% yield from 4-nitroanthraquinone-1-carboxylicacid. Refluxing anthraquinone-1-carboxylic acid in PhCl with PCl5 1 hr., followed by further heating 1 hr. with added p-O2NC6H4NHNH2 gave 40.2% yellow 1-(p-nitrophenyl)anthra-[9,1-cd]pyridazine-2,6-dione(II), m. 363-4°; the same was formed in 26.9% yield after similar reaction in 60% AcOH-KOAc solution without PCl5; or by the nitration of I with 98% HNO3 in concentrated H2SO4 1 hr. at 0-5°. Similarly was prepared 55.7% 1-(o-nitrophenyl)anthra[9,1-cd]pyridazine-2,6-dione,m. 265-6°; and 82.7% 1-(2,4-dinitrophenyl)anthra[9,1-cd]pyridazine-2,6-dione, m. 313-14.3°. Nitration of I with mixed acid as above gave 100% 4',7-dinitro derivative, m. 381-2°, also formed from the 7-nitro derivative of I and p-ClC6H4NO2; the reaction also gave an isomeric dinitro derivative, m. 319.7-20°. II was reduced with Na2S in aqueous EtOH in 4 hrs. to the p-aminophenyl analog, 83.6%, m. 317.8-19.2°; similarly was prepared 76.3% orange o-aminophenyl analog, m. 338-8.8°; and 100% red-brown 2,4-diaminophenyl analog, m. 329.5-31.3°. Anthraquinone-1,4-dicarboxylicacid and PhNHNH2 in 50% AcOH in the presence of KOAc refluxed 2 hrs. gave 60% 1,6-diphenylanthrabis[9,1-cd:10,4,c'd']pyridazine-2,6-dione(III), m. 381-2°, but with larger proportions of the dicarboxylic acid, the reaction gave 74% 1-phenylanthra[9,1-cd]pyridazine-2,6-dione-5-carboxyliacid, m. 388-9°. Bromination of I in AcOH, finally at reflux 2 hrs., gave 73.2% yellow 1-(p-bromophenyl)anthra[9,1-cd]pyridazine-2,6-dione,m. 308.5-9.3°.

IT 731-37-3, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione
(derivs.)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)

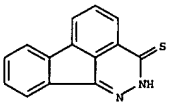


L4 ANSWER 28 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:476551 CAPLUS
DOCUMENT NUMBER: 61:76551
ORIGINAL REFERENCE NO.: 61:13305g-h,13306a-b
TITLE: 1,2-Diaza-2,3-dihydro-3-oxofluoranthenesobtained by cyclization of aryl and acylhydrazones of fluorenone-1-carboxylic acid and its esters. Conversion to 1,2-diaza-2,3-dihydro-3-thiocarbonylfluoranthene
AUTHOR(S): Quelet, Raymond; Dran, Raymonde; Lukacs, Gabor
CORPORATE SOURCE: Fac. Sci., Paris
SOURCE: Compt. Rend. (1964), 259(3), 590-3
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The following I were prepared by the method described previously (CA 60, 14448f) (R1, R2, and m.p. are given): Ph, H, 220°; o-O2NC6H4, Me (II), 170°; p-O2NC6H4, Me, 282°; 2,4(O2N)2C6H3, Me (III), 272°; Ac, H (IV), 242°; Bz, H (V), 248°. The cyclizations were achieved in about 80% yield by dissolving the various I in the min. amount of boiling AcOH. The solution volume was increased 60% by addition of Ac2O and the mixture refluxed 4 hrs. and evaporated to dryness in vacuo. The following VI were prepared [R and m.p. (crystallizing solvent) given]: H (VII), 268° (BuOAc); Me (VIII), 156° (alc.-H2O); Et (IX), 134° (alc.-H2O); Ph, 221° (AcOH); p-O2NC6H4, 324° (AcOH); Ac (X), 172° (C6H6-petr. ether); Bz (XI), 170° (C6H6-petr. ether). II and III yielded no product under these conditions, while IV and V were both converted to VII, from which X and XI were prepared by treatment with Ac2O and BzCl in C5H5N, resp., while VIII and IX resulted from the reaction of VII with MeI and EtI, resp., in alc. NaOH. The structure proposed for the unsubstituted derivative was confirmed by its infrared spectrum. Conversion of the various VI to the 3-thio derivs. (XII) was accomplished in 70-80% yield by refluxing them 2 hrs. with a mixture of a slight excess of P2S5 and xylene. The mixture was poured into H2O and the product separated by filtration or extraction. The following XII were prepared [R and m.p. (crystallizing solvent) given]: H, 263° (AcOH); Me, 165° (alc.); Et, 149°(alc.); Ph, 268° (AcOH); p-O2NC6H4, 287° (AcOH).

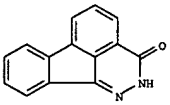
IT 36999-81-2, Indeno[1,2,3-de]phthalazine-3(2H)-one
58106-74-4, Indeno[1,2,3-de]phthalazine-3(2H)-thione
(derivs.)
RN 36999-81-2 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one(7CI, 8CI, 9CI) (CA INDEX NAME)



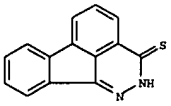
RN 58106-74-4 CAPLUS
CN Indeno[1,2,3-de]phthalazine-3(2H)-thione(7CI, 9CI) (CA INDEX NAME)



IT 36999-81-2F, Indeno[1,2,3-de]phthalazine-3(2H)-one
58106-74-4F, Indeno[1,2,3-de]phthalazine-3(2H)-thione
RL: PREP (Preparation)
(preparation of)
RN 36999-81-2 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one(7CI, 8CI, 9CI) (CA INDEX NAME)



RN 58106-74-4 CAPLUS
CN Indeno[1,2,3-de]phthalazine-3(2H)-thione(7CI, 9CI) (CA INDEX NAME)



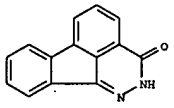
L4 ANSWER 29 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:476550 CAPLUS
DOCUMENT NUMBER: 61:76550
ORIGINAL REFERENCE NO.: 61:13305b-g
TITLE: Photochemical reactions of azo compounds. III. Photochemical cyclodehydrogenation of substituted

azobenzenes
AUTHOR(S): Badger, G. M.; Drewer, R. J.; Lewis, G. E.
CORPORATE SOURCE: Univ. Adelaide
SOURCE: Australian Journal of Chemistry (1964), 17(9), 1036-49
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

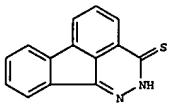
AB cf. CA 60, 8025c. The photocatalyzed cyclodehydrogenation of azobenzene (Lewis, CA 54, 21116a) and of methyl- and dimethylazobenzenes (CA 60, 8025c) were previously described. 2,4,6-Trimethylazobenzene (I) underwent photochem. cyclodehydrogenation in H2SO4 (with the loss of a Me group) to form 2,4-dimethylbenzo[c]cinnoline (II) and 1,3,4-trimethylbenzo[c]cinnoline (III) with migration of a Me group. A photochem. disproportionation was involved; 4-(4-aminophenyl)-2,4,6-trimethylcyclohexa-2,5-dienone (IV), formed by acid-catalyzed rearrangement and hydrolysis from I, was also isolated. I, red needles, m. 19.5°, was prepared by nitration of mesitylene, reduction with Sn and HCl, and condensation with PhNO in AcOH. A solution of 3 g. I in 145 ml. 20.5N H2SO4 was irradiated for 213 hrs. and the mixture diluted with H2O to 300 ml. and partially neutralized with 90 g. NaOH in 250 ml. H2O below 40°. Extraction with C6H6 yielded II, 20%, m. 121.5°, III, 2%, m. 146.5-7.5, and IV, 17%, m. 133.5-34°. A mixture of 96 mg. IV, 2.5 ml. Ac2O, and 0.1 ml. concentrated H2SO4 was kept for 21 hrs. at room temperature and then refluxed with 6 g. NaOH in 30 ml. H2O for 2 hrs. The mixture was acidified with HCl, buffered with Na2CO3 (pH 8), and extracted with ether to give 87 mg. 4-amino-3'-hydroxy-2',4',6'-trimethylbiphenyl, m. 163°. Substituted azobenzenes with a carboxy, iodo, or chloro group in the 4-, 3-, or 2-position were similarly irradiated. The resulting benzo[c]cinnolines and benzidines were isolated (m.p. given): Me benzo[c]cinnoline-2-carboxylate, (185.5°); benzo[c]cinnoline-2-carboxylic acid, 363-4° (in vacuo); 2-iodobenzo[c]cinnoline, 217.5-218°; benzidine, 122-3°; 2-iodobenzo[c]cinnoline N-oxide, 221.5-222.5°; 2-chlorobenzo[c]cinnoline, 215.5-216°; disalicylidenebenzidine, 258.5-260.5°; Me benzo[c]cinnoline-3-carboxylate, 177°; benzidine-2-carboxylic acid, 271.5-2.5° (in vacuo); 1-iodobenzo[c]cinnoline, 122°; 3-iodobenzo[c]cinnoline, 193-3.5°; N,N'-dibenzylidene-2-iodobenzidine, 157-7.5°; 1-chlorobenzo[c]cinnoline, 145-6°; 3-chlorobenzo[c]cinnoline, 189-90.5°; 2-chlorobenzidine, 101.5-2.5°; benzo[c]cinnoline-4-carboxylicacid, 283.5-85° (in vacuo); benzidine-3-carboxylic acid, 205-6° (in vacuo); 4-iodobenzo[c]cinnoline, 193.5-94°; 3-iodobenzidine, 70°; 4-chlorobenzo[c]cinnoline, 191-2°; 3-chlorobenzidine, 74.5-75°. Irradiation of 2-substituted azobenzenes gave the parent benzo[c]cinnoline as well as the 4-substituted benzo[c]cinnoline, which showed that carboxy, iodo, and chloro substituents could be ejected as well as Me. The irradiation of azobenzene-3-carboxylic acid gave 1-hydroxybenzo[c]cinnoline-10-carboxylicacid lactone, m. 329-30°, in addition to the benzo[c]cinnoline-3-carboxylicacid. Some biphenyls were prepared from 4-iodoazobenzene and 4-chloroazobenzene: 2,4'-diamino-5-iodobiphenyl, salicylidene derivative m. 150.5-1.5°, p-nitrobenzylidene derivative m. 215.5-216°; N,N'-di-salicylidene-5-chloro-2,4'-diaminobiphenyl, m. 167.5-68°; 5-chloro-2,4'-diaminobiphenyl, dibenzylidene derivative m. 105.5-6.5°. 20 references.

IT 36999-81-2, Indeno[1,2,3-de]phthalazine-3(2H)-one
58106-74-4, Indeno[1,2,3-de]phthalazine-3(2H)-thione
(deriva.)

RN 36999-81-2 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one(7CI, 8CI, 9CI) (CA INDEX NAME)

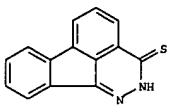


RN 58106-74-4 CAPLUS
CN Indeno[1,2,3-de]phthalazine-3(2H)-thione(7CI, 9CI) (CA INDEX NAMES)



IT 58106-74-4P, Indeno[1,2,3-de]phthalazine-3(2H)-thione
RL: PREP (Preparation)
(preparation of)

RN 58106-74-4 CAPLUS
CN Indeno[1,2,3-de]phthalazine-3(2H)-thione(7CI, 9CI) (CA INDEX NAME)



L4 ANSWER 30 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:454842 CAPLUS
DOCUMENT NUMBER: 61:54842
ORIGINAL REFERENCE NO.: 61:9494a-c
TITLE: Transformation of 3-hydrazinopyridazino[4,5,6-m,l]fluorene
AUTHOR(S): Dokunikhin, N. S.; Mikhalenko, S. A.
SOURCE: Zhurnal Obshchei Khimii (1964), 34(7), 2473-4
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

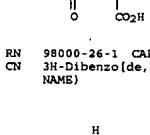
GI For diagram(s), see printed CA Issue.

AB 3-Chloropyridazino[4,5,6-m,l]fluoreneand N2H4.H2O gave the 3-hydrazino analog, isolated as the hydrate (I), which with HgO in alc. NaOH gave 80% pyridazino[4,5,6-m,l]fluorene (II), m. 123.6-25°; in the absence of HgO the yield was 54%. I, decomposed 255.6-56°, and 2 moles aqueous CuSO4 gave 85% 1-cyanofluorenone, m. 180-80.5°, also formed in 10% yield in alc. NaOH. Saponification with alc. alkali gave fluorenone-1-carboxylic acid. Similarly, 3-hydrazino-9-methylpyridazino[4,5,6-m,l]fluorene hydrate, m. 277.5-8.6°, gave 60% 1-cyano-7-methylfluorenone, m. 209.1-10°. I was unchanged by oxidizing agents such as Na2AsO4.

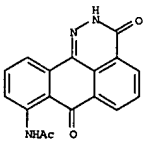
II picrate decomposed 221-2°.

IT 97594-69-9P, 3H-Dibenzo[de,h]cinnoline-6-carboxylicacid, 2,7-dihydro-3,7-dioxo 98000-26-1P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione, 8-acetamido-
RL: PREP (Preparation)
(preparation of)

RN 97594-69-9 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-6-carboxylicacid, 2,7-dihydro-3,7-dioxo- (7CI) (CA INDEX NAME)



RN 98000-26-1 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-acetamido- (7CI) (CA INDEX NAME)



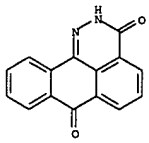
L4 ANSWER 31 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:454841 CAPLUS
DOCUMENT NUMBER: 61:54841
ORIGINAL REFERENCE NO.: 61:9493f-h,9494a
TITLE: Pyridazoneanthrone and its derivatives I
AUTHOR(S): Dokunikhin, N. S.; Fain, V. Ya.
SOURCE: Zhurnal Obshchei Khimii (1964), 34(7), 2372-4
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

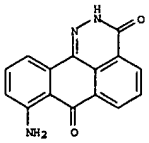
AB Refluxing anthraquinone-1-carboxylicacid in aqueous NaOAc in the presence of N2H4.H2SO4 7 hrs. gave 93% pyridazoneanthrone (I, R = H) (II), m. 426-7°; simple heating of the acid with N2H4.H2O 3 hrs. gave a 92.5% yield. Similar reaction of 4-aminoanthraquinone-1-carboxylicacid gave 85.7% 4-aminopyridazoneanthrone, decomposed 351.5-2.8°, also formed in 74.6% yield from 4-nitroanthraquinone-1-carboxylicacid refluxed 1 hr. with PCl5 in C6H6, then treated in the cold with N2H4.H2O 1 hr., followed by refluxing with dilute NH4OH; the use of N2H4.H2SO4 gave an 82.7% yield. II nitrated in concentrated H2SO4 with 98% HNO3 at 0° 1 hr. gave I (R = NO2), decomposed 291.2-3°, which with aqueous Na2S 1.5 hrs. at reflux gave 89% I (R = NH2), decomposed 372-3°, also formed in 91.5% yield from 5-aminoanthraquinone-1-carboxylicacid, via the route used above for preparation of II. I (R = NH2) was also formed by treatment of 5-nitroanthraquinone-1-carboxylicacid with PCl5 and N2H4, as shown above, the yield being 70.2%. The amine heated with Ac2O 0.5 hr. gave I (R = AcNH), decomposed 370-1°. Anthraquinone-1,4-dicarboxylicacid (III) heated successively with PCl5, then N2H4.H2O gave 92.5% anthra-1,4-dipyridazone (IV), decomposed about 500°. III in hot aqueous NaOAc was treated with N2H4.H2SO4 and refluxed 3 hrs. to yield 4% insol. IV, and 93.6% pyridazoneanthrone-4-carboxylicacid, decomposed 333.5-4.8°.

IT 731-37-3P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione
57981-26-7P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-amino-
57981-27-8P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-amino-
97216-39-2P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-nitro-
97594-69-9P, 3H-Dibenzo[de,h]cinnoline-6-carboxylicacid, 2,7-dihydro-3,7-dioxo 98000-26-1P, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione, 8-acetamido-
RL: PREP (Preparation)
(preparation of)

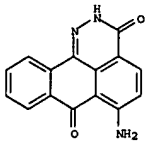
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



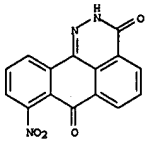
RN 57981-26-7 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-amino- (7CI, 9CI) (CA INDEX NAME)



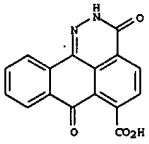
RN 57981-27-8 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,6-amino- (7CI, 9CI) (CA INDEX NAME)



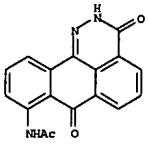
RN 97216-39-2 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-nitro- (7CI) (CA INDEX NAME)



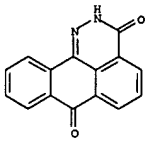
RN 97594-69-9 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-6-carboxylicacid, 2,7-dihydro-3,7-dioxo- (7CI) (CA INDEX NAME)



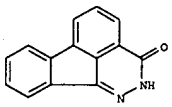
RN 98000-26-1 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione,8-acetamido- (7CI) (CA INDEX NAME)



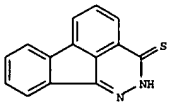
L4 ANSWER 32 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:454840 CAPLUS
DOCUMENT NUMBER: 61:54840
ORIGINAL REFERENCE NO.: 61:9493e-f
TITLE: Action of nitric acid on polybromophenothiazines
AUTHOR(S): Bodea, Cornel; Farcasan, V.; Oprean, I.
CORPORATE SOURCE: Chem. Inst., Cluj, Rom.
SOURCE: Zhurnal Obshchei Khimii (1964), 34(7), 2369-71
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 55, 550b. Nitration of polybromophenothiazine-5,5-dioxidesin fuming HNO3 with ice cooling, followed by 12 hrs. at room temperature, gave the following products: 1,9-dibromo-3,7-dinitrophenothiazine5,5-dioxide, m. 305°, formed from 1,3,7,9-tetrabromophenothiazinedioxide or 1,3,7,9-tetrabromophenothiazine;1,3,7,9-tetranitrophenothiazine 5,5-dioxide, m. 344-5°, formed from 3,7-dibromophenothiazine 5,5-dioxide, or 3,7-dibromophenothiazine;1-bromo-3,7,9-trinitrophenothiazine5,5-dioxide, m. 311-12°, formed from 1,3,7-tribromophenothiazine5,5-dioxide or 1,3,7-tribromophenothiazine; 1-nitro-3,7-dibromophenothiazine5,5-dioxide, m. 297-8°, formed from 3,7-dibromophenothiazine5,5-dioxide by heating with fuming HNO3 in AcOH 2 min. at reflux.
IT 731-37-3F, 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione
RL: PREP (Preparation)
(preparation of)
RN 731-37-3 CAPLUS
CN 3H-Dibenzo[de,h]cinnoline-3,7(2H)-dione(7CI, 8CI, 9CI) (CA INDEX NAME)



L4 ANSWER 33 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:454962 CAPLUS
DOCUMENT NUMBER: 59:54962
ORIGINAL REFERENCE NO.: 59:10037b-g
TITLE: 1,9-Substituted derivatives of fluorene. I. Synthesis and transformations of 2H,3H-pyridazino[4,5,6-m,n]fluoren-3-one
AUTHOR(S): Dokunikhin, N. S.; Mikhalenko, S. A.
SOURCE: Zhurnal Obshchei Khimii (1963), 33(6), 1974-7
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Treating fluorenone-1-carboxylic acid (Ia) with excess N2H4.H2O, gave 2H,3H-pyridazino[4,5,6-m,n]fluoren-3-one(I). Ia with an equimolar amount N2H4.H2O gave Ia hydrazone (II), which could be cyclized to I. I could also be prepared from the Me ester (III) of II or treating semiearbazide with Ia. I with P2S5 gave 2H,3H-pyridazino[4,5,6-m,n]fluorene-3-thione (IV), which formed with substituted 3-hydroxythionaphthenes dyes (V) analogous to those derived from benzo[c,d]indole. II with BzH gave the 9-benzylidenehydrazone (VI) of Ia. Ia (1.12 g.) and 0.27 ml. N2H4.H2O in 40 ml. alc. was refluxed 20 min., cooled, filtered off and the product washed with alc. to give 0.98 g. yellow II, m. 218-20.5° (decomposition) (AcOH), γ 250 mμ (AcOH). II (1.4 g.) and 2.0 g. BzH in 40 ml. Bu alc. was refluxed 3 hrs. and 30 ml. BuOH distilled The precipitate that formed on cooling was washed with a small amount BuOH to yield 2.0 g. VI, yellow, m. 220.6-2.5° (C6H6). Ia Me ester (1.4 g.) was added at 55° to a solution of 1.0 g. N2H4.H2O in 12 ml. alc., brought to pH 5.5 with H2SO4, BaCO3 added to pH 5-6, the mixture stirred 40 min. at 50-5°, cooled, the precipitate filtered off and extracted with alc., and the alc. solution evaporated to dryness to yield 1.44 g. III, m. 131.5-33° (decomposition) (Et2O), bright yellow. Ia (2.24 g.) and 2.5 ml. N2H4.H2O in 300 ml. alc. was refluxed 2 hrs., 150 ml. alc. distilled, the mixture diluted with H2O, cooled, filtered off, and the precipitate washed with H2O, treated with 10% NH4OH, filtered off, and dried to yield 1.54 g. I, m. 270.5-72° (PhCl), γ 257 mμ, (AcOH). I was also prepared by boiling Ia and N2H4.H2O in AcOH in the presence of NaOAc; by boiling HI in an NaOH solution; by boiling III in AcOH; by boiling II in AcOH with NaOAc; and by treating Ia with semicarbazideHCl in AcOH at 70-5°. Bz derivative of I m. 190-1° (EtOH); Ac derivative of I (by boiling I in Ac2O) m. 177-8° (EtOH). I and 2.5 g. P2S5 in 10 ml. C5H5N was refluxed 20 hrs., the mixture diluted with H2O, and the precipitate washed with H2O, dilute HCl, and H2O to yield 2.2 g. crude IV, 1.32 g. after 2 extns. with o-xylene m. 253.5-5.2° (C6H6-MeOH). IV (0.47 g.) and 0.4 g. 6-chloro-3-oxobenzothiophene in 30 ml. trichlorobenzene was refluxed 30 hrs. (until evolution of H2S ceased), the mixture cooled, and the precipitate filtered off, washed with alc., and dried. This product (0.5 g.) was extracted with alc. and treated with an alkaline hydrosulfite solution to yield 0.46 g. V (X = 6-Cl), red crystals from trichlorobenzene, m. 832-3.5°. V (X = 4,5-benzo) was prepared similarly from IV and 4,5-benzo-3-oxobenzothiophene, red, m. 324-5°. Also prepared was V (X = 6-EtO), red, m. 289.4-93° (trichlorobenzene, o-xylene)
IT 36999-81-2F, Indeno[1,2,3-de]phthalazino-3(2H)-one
58106-74-4F, Indeno[1,2,3-de]phthalazine-3(2H)-thione
RL: PREP (Preparation)
(preparation of)
RN 36999-81-2 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one(7CI, 8CI, 9CI) (CA INDEX NAME)



RN 58106-74-4 CAPLUS
CN Indeno[1,2,3-de]phthalazine-3(2H)-thione(7CI, 9CI) (CA INDEX NAME)



L4 ANSWER 34 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:46565 CAPLUS
DOCUMENT NUMBER: 58:46565
ORIGINAL REFERENCE NO.: 58:7882b-h,7883a-h,7884a-h
TITLE: 3-Hydroxyfluoranthene-1-, -2-, and -10-carboxylic acids
AUTHOR(S): Sieglitz, Adolf; Troester, Helmut; Boehme, Peter
CORPORATE SOURCE: Tech. Hochschule, Munich, Germany
SOURCE: Chemische Berichte (1962), 95, 3013-29
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Carboxylic acid derivs. of 3-oxo-1,2,3,10b-tetrahydrofluoranthene(I) are converted by treatment with air in alkaline medium into the corresponding 3-hydroxyfluoranthenecarboxylicacids and their derivs. The irradiation of 3-hydroxyfluoranthene (II) yielded 1-carboxyfluorene-9-acetic acid (III); the 3-hydroxyfluoranthene-1-carboxylicacid (IV) gave in an analogous manner 1-carboxy-9-fluorenylmalonicacid (V). Fluorene (VI) (332 g.) and 98 g. maleic anhydride (VII) atirred 24 hrs. at 200°, poured into 120 g. Na2CO3 in 1.5 l. H2O, the mixture refluxed 0.5 hr., filtered hot, the residue boiled twice with dilute aq. Na2CO3 and filtered, and the combined filtrates acidified with concentrated HCl and filtered yielded 160-90 g. 9-fluorenylsuccinic acid (VIII), m. 186° (40% AcOH); VIII esterified with EtOH and H2SO4 gave the di-Et ester, m. 63-4° (EtOH). VIII (282 g.) and 800 cc. Ac2O refluxed 3 hrs., cooled, and filtered yielded 218 g. anhydride (IX) of VIII, m. 168°. IX (13.2 g.) and 9.3 g. PhNH2 heated to boiling, cooled, triturated with 2N HCl, and filtered yielded 17 g. anilic acid, m. 186-7° (EtOH). IX (264 g.) added during 15 min. with stirring at 130° to 467 g. AlCl3 and 175 g. NaCl, the whole kept 5 min. at 130°, cooled, treated with 300 cc. H2O and 250 cc. concentrated HCl, and filtered gave 263 g. cis-trans-mixture of the 1-CO2H derivative (X) of I; a 75-g. portion recrystd. from 450 cc. AcOH yialded 35.5 g. cis-X, m. 237-40°; Et ester m. 103.5-4.5° (EtOH); the mother liquor boiled with 450 cc. H2O, filtered, cooled, and again filtered, the dried residue (29 g.) refluxed 1 hr. with 150 cc. MeOH and 10 cc. concentrated H2SO4, cooled, and filtered, and the Me ester (15.2 g.), m. 135°, of trans-X refluxed 8 hrs. with 200 cc. 40% H2SO4, diluted with 200 cc. H2O, cooled, and filtered yielded 14

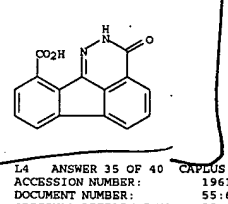
162(b).

g. trans-X, m. 208° (AcOH). cis-X heated 15 min. at 260° gave a cis-trans-X mixture cis-X (2 g.) in 15 cc. warm 1.5N Na2CO3 kept 0.5 hr. at 90°, poured into 15 cc. 20% AcOH, and the whole refrigerated gave 1.7 g. trans-X, m. 207-8° (50% AcOH). trans-X (4 g.), 28 g. Cu powder, and 56 g. BaO heated slowly to 280° gave fluoranthene (XI), m. 109-10°. trans-X esterified with EtOH-H2SO4 yielded the Et ester, m. 88-9° (EtOH). trans-X (1.4 g.) refluxed with SOCl2 and evaporated, and the residue heated 1 hr. on a water bath with concentrated NH4OH and filtered yielded 0.7 g. 1-CONH2 derivative (XII) of I, needles, m. 248-50° (EtOH). trans-X (26.4 g.) and 9.3 g. PhNH2 in 1200 cc. xylene treated dropwise with stirring with 6.8 g. PCl3 in 50 cc. xylene, the mixture refluxed 4 hrs., treated with 100 cc. 2N Na2CO3, steam distilled to remove the xylene, and the residue cooled and filtered yielded 19 g. 1-CONHPh derivative (XIII) of I, m. 229-31° (PhCl or 70% AcOH), also obtained from cis-X. trans-X (1.32 g.), 0.35 g. NH2OH.HCl, and 0.7 g. NaOAc in 30 cc. 80% EtOH refluxed 8 hrs. gave the oxime, m. 240-2° (decomposition) (EtOH), also obtained from cis-X; semicarbazone m. 250-2° (decomposition) (EtOH); also obtained from cis-X. cis-trans-X (26.4 g.) in 500 cc. 2N NaOH treated 1 hr. with stirring and aerating on a steam bath, and the mixture acidified with concentrated HCl, cooled, and filtered yielded 24.9 g. IV, m. 261-2° (AcOH). IV distilled with Zn dust gave XI. IV (2.6 g.), 1.5.g. Cu powder, and 30 cc. quinoline refluxed 1 hr., or 2.6 g. IV and 100 g. 100% H3PO4 heated 0.5 hr. at 275° did not give II. IV (2.6 g.), 20 cc. Ac2O, and 2.6 g. NaOAc refluxed 4 hrs., the mixture concentrated to 1/3 of the original volume, decomposed with H2O, and filtered yielded 3 g. acetate of IV, m. 236° (AcOH). IV gave in the usual manner a Me ester, m. 235-6° (MeOH), and an Et ester (XIV), m. 213-14°. XII (2.6 g.) in 50 cc. EtOH, 150 cc. H2O, and 50 cc. 2N NaOH aerated 5 hrs. with stirring on a water bath, the whole filtered, acidified with dilute H2SO4, filtered, and the dried residue (2 g.) recrystd. from 10 cc. AcOH and twice from 50 cc. 50% EtOH gave the 1-CONH2 derivative of II, m. 273° (50% EtOH). XIII (17 g.), 1700 cc. 50% EtOH, and 170 cc. 2N NaOH aerated 7 hrs., diluted with 500 cc. H2O, and acidified with 150 cc. AcOH gave 19 g. 1-PhNHCO derivative (XV) of II, m. 260°. IV(13.1 g.)in 200 cc. 2N NaOH treated with stirring with 25 g. Me2SO4 and the mixture filtered yielded 9.3 g. Me ester (XVI) of 3-methoxyfluoranthene-1-carboxylic acid,(XVII), m. 157-8° (AcOH). XVI (2.9 g.), 50 cc. MeOH, and 100 cc. 2N NaOH refluxed 12 hrs., the mixture filtered, acidified with concentrated HCl, filtered, and the residue refluxed with 600 cc. AcOH, filtered, concentrated to 200 cc. I cooled, and filtered gave 2.5 g. (crude) XVII, m. 301-3°. XVI, (1 g.), 0.5 g. Cu powder, and 10 cc. quinoline refluxed 0.5 hr., the mixture cooled, diluted with 50 cc. Et2O, filtered, diluted with 100 cc. Et2O, and worked up gave 0.65 g. 3-methoxyfluoranthene, m. 157° (EtOH). IV (0.75 g.) in 400 cc. N NaOH irradiated 19 days with a 200-w. bulb, the mixture filtered, acidified with concentrated HCl, and filtered after 1 week gave V, m. 231-4° (upon slow heating), 220° (decomposition) (upon rapid heating) (dilute AcOH). V (0.5 g.) in 10 cc. AcOH treated dropwise with 1.5 g. CrO3 in 5 cc. 50% AcOH, the mixture refluxed 12 hrs., poured into dilute H2SO4, and filtered gave fluorenone-1-carboxylic acid, m. 194-5° (aqueous AcOH). V (0.5 g.) heated 10 min. at 220-30° gave 0.3 g. III, m. 232-4° (dilute AcOH). II (1 g.) in 800 cc. N NaOH irradiated 14 days, and the mixture filtered and acidified with concentrated HCl yielded 1.0 g. III, m. 231-2° (50% AcOH). 2-COCO2Me derivative (0.5 g.) of I in 10 cc. AcOH and 8 cc. 40% H2SO4, refluxed 1 hr., the mixture cooled, treated with 3 cc. 30% H2O2, the whole heated carefully until gas evolution began, kept several days, and filtered yielded 0.15 g. III, m. 230-2° (50% AcOH). II (0.44 g.) and 2 g. NaOAc in 40 cc. 0.5N NaOH treated dropwise with stirring and cooling with the filtered solution of 1.6 g. Echtrosalz GG (XVIII) (= 1.8 millimoles p-nitrobenzenediazoniumsalt) in 40 cc. 0.25N AcOH, and filtered gave 0.5 g. 2-(p-O2NC6H4N2) derivative (XIX) of II, m. 302-3° (decomposition) (xylene). 2-CO2H derivative (XX) (0.1 g.) of II in 10 cc. 2N NaOH and 50 cc. H2O, neutralized with 2N NaOH, coupled in the usual manner with XVIII, and the mixture stirred 2 hrs., heated 1 hr. at 60°, and filtered gave 0.12 g. XIX, m. 302-3° (xylene). IV (1.3 g.) in 10 cc. 2N NaOH and 30 cc. H2O neutralized with 2N AcOH, coupled with cooling with 5 millimoles; XVIII in 50 cc. H2O and 1 cc. AcOH, stirred 6 hrs., and filtered gave 1.7 g. 2-(p-nitrophenylazo)-3-hydroxyfluoranthene-1-carboxylicacid (XXI), m. 350-5° with previous darkening (decomposition) (EtOH and then MeOCH2CH2OH). XIV (1.45 g.) in 20 cc. C5H5N treated with stirring and cooling with 5 millimoles XVIII, and the whole stirred 6 hrs. at room temperature and poured into 300 cc. H2O yielded the Et ester of XXI, m. 265-70° (AcOH). 4,2-Me(O2N)C6H3NH2 (40 millimoles) diazotized, filtered, added with stirring to 14.2 g. XV, 3.3 g. NaOAc, 40 cc. 2N NaOH, and 100 cc. Me2CO at 20°, and the mixture heated 0.5 hr. at 60-70°, cooled, and filtered yielded 19.8 g. 2-(4-methyl-2-nitrophenylazo)-3-hydroxyfluoranthene-1-carboxanilide (XXII), m. 291-3° (decomposition) (xylene). VI (49.8 g.) in 200 cc. propylene oxide treated with stirring and cooling during 2 hrs. with 47 g. Cl and the mixture evaporated on a water bath gave 36.1 g. 2,7-dichlorofluorene (XXIII), m. 125-6° (EtOH). XXIII (235 g.) and 98 g. VII heated 45 hrs. at 210-30° gave about 50% unchanged XXIII and 80-100 g. (crude) 2,7-dichloro-9-fluorenylsuccinicacid (XXIV), m. 223° (75% AcOH); di-Me ester m. 149-9.5° (MeOH). Crude XXIV refluxed 2 hrs. with 4 parts Ac2O, and the mixture concentrated to 1/4 of the original volume, kept several days, and filtered yielded 90% (crude) anhydride (XXV) of XXIV, m. 206-7° (C6H6). Crude XXV (83 g.) added during 25 min. in portions with stirring to 200 g. AlCl3 and 88 g. NaCl at 140-50°, stirred 10 min., decomposed with H2O and dilute HCl, and filtered yielded 82 g. cis-trans-mixture of 4,9-dichloro-3-oxo-1,2,3,10b-tetrahydrofluoranthene-1-carboxylic acid (XXVI). Crude XXVI (82 g.) recrystd. slowly from 700 cc. AcOH gave 42 g. (crude) cis-XXVI, m. 232-3°. cis-XXVI (3.3 g.) in 175 cc. refluxing MeOH treated dropwise during 0.5 hr. with 17.5 cc. concentrated H2SO4, and the mixture refluxed 75 min., distilled to remove 75 cc. MeOH, and cooled yielded 2.9 g. Me ester of cis-XXVI, m. 182°, which, recrystd. from MeOH, yielded the trans-Me ester, m. 170-2°. Me ester (0.5 g.) of trans-XXVI refluxed 6 hrs. with 20 cc. 50% H2SO4 gave 0.45 g. trans-XXVI, m. 252-3°. The AcOH mother liquor from the crude cis-XXVI refluxed with 700 cc. H2O, and the crude product (33 g.) repeatedly recrystd. from AcOH yielded trans-XXVI, m. 252-3° (PhCl); Me ester m. 172.5-73° (MeOH). XXVI heated with 2N NaOH and acidified with AcOH gave the 4,9-di-Cl derivative of IV, m. 293-4° (decomposition) (AcOH); Et ester m. 188-9° (EtOH). cis- or trans-XXVI (3.3 g.) in 200 cc. refluxing AcOH treated dropwise with 15 g. Na2Cr2O7 in 150 cc. H2O and 15 cc. concentrated H2SO4 during 45 min., the mixture refluxed 5 hrs., poured into 1 l. H2O, filtered, and the residue repptd. from aqueous Na2CO3 with HCl gave 1.6 g. 2,7-dichlorofluorenone-1-carboxylicacid, m. 256-8° (50% AcOH). VI (166 g.) in 1500 cc. propylene oxide treated at room temperature with stirring during 3 hrs. with 60 cc. Br, and the mixture stirred 4 hrs. and evaporated gave 88 g. 2-bromofluorene (XXVII), m. 112-13° (EtOH) (38.6 g. 2nd crop). XXVII treated with VII as described for XXIII during 32 hrs. at 200° gave 12% 2-bromo-9-fluorenylsuccinicacid (XXVIII), m. 218° (80% AcOH), and about 65% unreacted XXVII; anhydride (XXIX) of XXVIII m. 150-2°. XXIX (9.7 g.), 13.2 g. AlCl3, and 5 g. NaCl gave in the usual manner 9.2 g. 9-bromo-3-oxo-1,2,3,10b-tetrahydrofluoranthene-1-carboxylicacid (XXX), m. 210-30°. Crude XXX (9.2 g.) recrystd. from 15 cc. boiling AcOH and then twice from a 10-fold amount AcOH gave cis-XXX, m. 243-5°; the mother liquor diluted with an equal volume H2O, and the precipitate recrystd. from 50% AcOH gave an addnl. 1.4 g. cis-XXX. cis-XXX (0.3 g.) in 100 cc. N Na2CO3 heated under N 0.5 hr. on a water bath, and the mixture poured into 50 cc. 25% HCl and filtered yielded trans-XXX, m. 233° (50% AcOH). cis-XXX (1.8 g.) in 300 cc. N NaOH aerated 1.5 hrs. on a steam bath, and the mixture acidified with concentrated HCl and filtered yielded 1.8 g. (crude) 9-bromo-3-hydroxyfluoranthene-1-carboxylicacid (XXXI), m. 288-9° (AcOH), m. 265° (MeOH). Me2SO4 (10 cc.) added dropwise with stirring at room temperature to 0.5 g. XXXI in 50 cc. 2N NaOH, and the mixture stirred 2 hrs. and filtered yielded 0.5 g. Me ester (XXXII) of 9-bromo-3-methoxyfluoranthene-1-carboxylicacid (XXXIII), m. 170-1° (AcOH). XXXII (160 mg.) refluxed 2 hrs. with 10 cc. AcOH, 2 cc. H2O, and 1 cc. concentrated H2SO4 gave XXXIII, m. 274-5° (AcOH). cis-XXX (0.5 g.), 3 g. Na2Cr2O7, 30 cc. AcOH, 10 cc. H2O, and 2 cc. concentrated H2SO4 refluxed 2 hrs., and the mixture poured into 300 cc. H2O and filtered yielded 7-bromofluorenone-1-carboxylicacid, m. 230-2° (70% AcOH). Na (0.92 g.) in 10 cc. absolute MeOH evaporated in vacuo on a water bath, the residue powdered, refluxed about 10 min. with 4.72 g. (CO2Me)2 and 20 cc. dry C6H6, the mixture cooled, treated under N with 4.4 g. I and 30 cc. dry C6H6, stirred 5 hrs. under N, treated with 240 cc. H2O, a small amount of ice and 2% aqueous NaOH, the C6H6 layer extracted with 50 cc. 2% aqueous NaOH, and the combined aqueous alkaline solns. filtered, acidified with dilute HCl, and refrigerated 2 days gave 5.57 g. 2-COCO2Et derivative (XXXIV) of I, m. 124-6° (decomposition) (1:1 Me2CO-MeOH). XXXIV (10 g.) heated above its m.p. until CO evolution began, treated with 5 g. glass powder, heated during 1 hr. to 180-90°, cooled, dissolved in 150 cc. Me2CO, and the solution decanted from the glass powder, concentrated to 50 cc., diluted with 50 cc. MeOH, treated with C, and refrigerated gave 7.4 g. 2-CO2Me derivative (XXXV) of I, m. 135-7.5° (1:1 MeOH-Me2CO). XXXV (1.4 g.) in 50 cc. AcOH refluxed 2 hrs. with 0.5 g. PhNHNH2, and the mixture poured into 200 cc. iced H2O, and filtered gave 1.2 g. 1'-phenyl-5'-oxopyrazolino[3',4':3,2]-1,2,3,10b-tetrahydrofluoranthene, m. 290° (decomposition) (EtOH). XXXV (6 g.) in 400 cc. EtOH treated dropwise during 15 min. on a steam bath with stirring and aerating with 1:1 2N NaOH-EtOH, and the mixture aerated another 10 min. with stirring, diluted with 200 cc. H2O, acidified hot with AcOH, and filtered yielded 1.4 g. Me ester (XXXVI) of 3-hydroxyfluoranthene-2-carboxylicacid (XXXVII), m. 146-8° (MeOH). XXXVI (1 g.) in 60 cc. AcOH treated during 1 hr. dropwise with 25 cc. 50% H2SO4, refluxed 4 hrs., and the mixture poured into 200 cc. iced H2O and filtered yielded 0.5 g. XXXVII, m. 230° (decomposition from 205°) (80% AcOH). XXXV (10 g.), 150 cc. MeOH, and 200 cc. 10N KOH refluxed 2.5 hrs. under N, and the mixture cooled, filtered, treated with C, and acidified with concentrated HCl gave 6.5 g. 1-carboxyfluorene-9-propionicacid (XXXVIII), m. 236-8° (decomposition) (70% AcOH); di-Me ester m. 50-2° (MeOH). XXXVIII (21.15 g.) and 90 cc. SOCl2 refluxed 1 hr. and evaporated, the residue in 42 cc. PhNO2 added dropwise with stirring and cooling during 1 hr. to 42 g. PhNO2 in 225 cc. PhNO2 at 6°, and the mixture refrigerated 2 days, poured into 60 cc. concentrated HCl and 800 g. ice, the PhNO2 layer washed with H2O and distilled with steam, the residue filtered, the crude filter residue (19.75 g.) dissolved in 200 cc. AcOH and filtered, the filter sludge boiled twice with 75 cc. AcOH each time, and the combined AcOH solns. diluted with 40 cc. H2O, treated with C, and cooled gave 14.5 g. 10-CO2H derivative (XXXIX) of I, m. 260-1° (50% AcOH); Me ester m. 140-1° (MeOH); Et ester m. 136-7.5° (EtOH); oxime m. 285-90° (decomposition) (MeOH). XXXIX in N NaOH aerated, acidified after 0.5 hr. with concentrated HCl, and filtered gave 94% 10-CO2H derivative (XL) of II, m. 271-2° (50% EtOH and then o-C6H4Cl2); Me ester m. 164° (60% MeOH); Et ester m. 163° (50% EtOH). XL with Me2SO4 in aqueous NaOH gave the Me ester (XLI) of 3-methoxyfluoranthene-10-carboxylicacid (XLII), m. 129-30° (MeOH). XLI refluxed 24 hrs. with 10N NaOH in MeOH and filtered, and the residue boiled 20 min. with 20% HCl gave XLII, m. 292-3° (EtOH), which was converted in the usual manner to the 2-(p-O2NC6H4N:N) derivative of XLII.AcOH, m. 328-9°, which, dried in vacuo at 180°, gave the solvent-free product, m. 328-9°. XXXIX (2.64 g.) in 180 cc. refluxing AcOH treated dropwise during 45 min. with 15 g. Na2Cr2O7 in 25 cc. H2O and 10 cc. concentrated H2SO4, the mixture refluxed 4 hrs., poured into 700 cc. H2O, kept overnight, and filtered gave 1.15 g. fluorenone-1,8-dicarboxylicacid (XLIII), m. 328-9° (AcOH). 1,1'-(4,4'-Dioxo-1,2,3,4,1',2',3',4'-octahydro-8,8'-binaphthyl)spirane (5.2 g.) in 150 cc. AcOH, 30 g. Na2Cr2O7, 30 cc. concentrated H2SO4, and 40 cc. H2O refluxed 3 hrs. yielded 1.65 g. crude XLIII; di-Me ester m. 178-9° (MeOH); di-Et ester m. 138-9° (50% EtOH). XLIII (0.5 g.), 30 cc. dioxane, and 3 cc. 80% N2H4.H2O refluxed 1 hr., cooled, and filtered gave 0.5 g. 3-hydroxy-1,2-diazafluoranthene-10-carboxylicacid, m. 375-6° (AcOH).

IT 97339-26-9F, Indeno[1,2,3-de]phthalazine-10-carboxylicacid, 3-hydroxy-
RL: PREP (Preparation)
(preparation of)

RN 97339-26-9 CAPLUS

CN Indeno[1,2,3-de]phthalazine-10-carboxylic acid, 3-hydroxy- (7CI) (CA INDEX NAME)



102(b). Cl. 14,
WHERE BOTH q = ϕ, Y = N, X = A BOND, R9 = H.

L4 ANSWER 35 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1961:67720 CAPLUS
DOCUMENT NUMBER: 55:67720
ORIGINAL REFERENCE NO.: 55:12867e-i,12868a-d
TITLE: Anthradipyridazones and their use in polymeric materials as optical bleaching agents
INVENTOR(S): Irving, Francis; Reece, Charles H.; Munro, Neil; Wilson, Robert H.
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 838994		19600622	GB 1956-37142	19561205
DE 1060403			DE	
US 2992220		19610711	US 1957-699440	19571129

GI For diagram(s), see printed CA Issue.

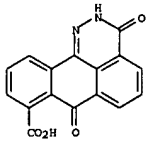
AB Anthra-1'9'(N),10',(N),4'(or5')-dipyridazones of the general formula I, where X and Y are H or univalent organic radicals, are useful as optical bleaching agents for high polymers such as poly(ethylene terephthalate), poly(hexamethyleneadipamide), polycaprolactam, and cellulose acetate. The bleaching agents may be added to the polymer which is then melted and cast or spun, or the compds. may be mixed with the monomers prior to polymerization as in the case of poly(ethylene terephthalate). For example, 2 parts 2-butyl-anthra-1',9'(N)-pyridazone-5'-carboxylicacid (II) and 1 part 2,6-Me2C6H3NH NH2 were heated at 220° for 30 min., cooled, stirred with 100 parts boiling 1% aqueous NaOH, filtered, the precipitate stirred with 100 parts 1% HCl, and filtered to give pale yellow 2-(2,6-dimethylphenyl)-8-butylanthra-1',9'(N),10'-(N),5'-dipyridazonem. 198-200° (EtOH). 1,5-Anthraquinonedicarboxylicacid (10 parts), 3 parts BuNHNH2, and 1.3 parts NaOH were heated at 200° for 15 min., cooled, stirred with 200 parts boiling 1% aqueous NaOH, filtered, 20 parts

NaCl added to the filtrate, filtered, the precipitate dissolved in 300 parts H2O, and acidified to precipitate II, m. 250°. Similarly prepared were the following agents and intermediates (color and m.p. given): 2-(2,6-dimethylphenyl)anthra-1',9'(N)-pyridazone-5'-carboxylicacid, pale yellow, 310-12°; 2,8-diphenylanthra-1',9'(N),10'(N),5'-dipyridazone, greenish yellow, 391-3° [o-ClC6H4 (III)]; 2,8-di-p-tolylanthra-1',9'(N),10'(N),5'-dipyridazone,-, <390°; 2,8-bis(2-chlorophenyl)anthra-1',9'(N),10'(N),5'-dipyridazonepale yellow 400°; 2,8-bis(2,5-dichlorophenyl)anthra-1',9'(N), 10'(N),5'-dipyridazone, pale yellow, 432°; 2,8-dibutyl-anthra-1',9'(N),10'(N),5'-dipyridazone, yellow, 185-6° (EtOH); 2,7-diphenylanthra-1',9'(N),10'(N),4'-dipyridazone,light greenish yellow, 394.5-6° (III); anthra-1',9'(N),10'(N),5'-dipyridazone,light brown, >400°; 2,8-bis(2,6-dimethylphenyl)anthra-1',9'(N),10'(N),5'-dipyridazone, light yellow, 369° (III); 2,8-bis(2-hydroxyethyl)anthra-1',9'(N),10'(N),5'-dipyridazone,yellow, 307° (III); 2-(2,6-dimethylphenyl)anthra-1',9'(N),10'(N),5'-dipyridazone-, 348-50° (III); 2,8-bis(2,6-diethylphenyl)anthra-1',9'(N),10'(N),5'-dipyridazone, pale yellow, 362°; 2-(2,6-diethylphenyl)anthra-1',9'(N),10'(N),5'-dipyridazone,-, 300°; 2,8-bis(o-bromophenyl)anthra-1',9'(N),10'(N),5'-dipyridazone,cream, -; 2-(6-chloro-2-methylphenyl)anthra-1',9'(N),10'(N),5'-dipyridazone, -, 349°; 2-(6-chloro-2-methylphenyl)anthra-1',9'(N)-pyridazone-5'-carboxylic acid, pale yellow, 305°; 2-(2,6-dichlorophenyl)anthra-1',9'(N),10'(N),5'-dipyridazone, yellow, 379° (III); 2-(2,6-dichlorophenyl)anthra-1',9'(N)-pyridazone-5'-carboxylicacid, pale gray, 325°; anthra-1',9'(N)-pyridazone-5'-carboxylicacid, yellow, 389°; 2-(2,6-dimethylphenyl)-7-butylanthra-1',9'(N)10'(N),4'-dipyridazone, pale yellow, 240-2°; 2-(2,6-dimethylphenyl)-anthra-1',9'(N)-pyridazone-4'-carboxylicacid, yellow, 283-7°; 2,7-dibutylanthra-1',9'(N),10'(N),4'-dipyridazone,pale yellow, 183° (III); 2,7-bis(o-chlorophenyl)anthra-1',9'(N),10'(N),4'-dipyridazone, pale cream, 412-14°; and 2,7-bis(2,6-dimethylphenyl)anthra-1',9'(N),10'(N),4'-dipyridazone, pale yellow, 358°.

IT 132647-76-8F, 7H-Dibenzo[de,h]cinnoline-8-carboxylicacid, 2,3-dihydro-3,7-dioxo-
RL: PREP (Preparation)
(preparation of)

RN 132647-76-8 CAPLUS

CN 7H-Dibenzo[de,h]cinnoline-8-carboxylicacid, 2,3-dihydro-3,7-dioxo- (6CI) (CA INDEX NAME)



L4 ANSWER 36 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1960:118310 CAPLUS

DOCUMENT NUMBER: 54:118310

ORIGINAL REFERENCE NO.: 54:22647h-i,22648a

TITLE: Synthesis of some aza- and diazafluoranthene derivatives

AUTHOR(S): Campbell, N.; Reid, K. F.; White, J. A.

CORPORATE SOURCE: Univ. Edinburgh, UK

SOURCE: Chemistry & Industry (London, United Kingdom) (1960) 494
CODEN: CHINAG; ISSN: 0009-3068

DOCUMENT TYPE: Journal

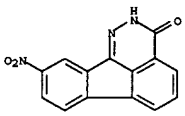
LANGUAGE: Unavailable

AB Fluorenone-1-(o-benzoyl chloride) (1 g.) in 23 ml. dry Me2CO at 0-5° treated with 0.3 g. NaN3 in 1 ml. H2O, the solution extracted with Et2O, the extract concentrated, 25 ml. concentrated HCl added, the solution heated slowly to 100°, boiled 15-30 min., poured into aqueous KOH, the solid extracted with Et2O, the organic layer washed free of KOH, dried (Na2SO4), and the Et2O removed gave 0.71 g. 6-aza-4,5-benzoacephenanthrylene(I), m. 168-9°, λ 373.5, 352.5, 341, 301, 289, 280.5, 262, 257 (inflection), 234, 229 mμ, log ε 3.67, 3.91, 3.98, 4.43, 4.40, 4.46, 4.59, 4.55, 4.58, 4.56 (hexane). I was weakly basic and could be extracted from concentrated HCl with CHCl3. 7-Nitrofluorenone-1-carboxylic acid with (H2N)2 in boiling dioxane gave 3-hydroxy-9-nitro-1,2-diazafluoranthene, m. above 350°. Similarly, 3,4-benzofluorenone-1-carboxylic acid gave 5-hydroxy-3,4-diaza-1,2-benzanthrylene,m. above 350°.

IT 36993-60-9F, Indeno[1,2,3-de]phthalazin-3-ol,9-nitro-
RL: PREP (Preparation)
(preparation of)

RN 36993-60-9 CAPLUS

CN Indeno[1,2,3-de]phthalazin-3(2H)-one,9-nitro- (9CI) (CA INDEX NAME)



L4 ANSWER 37 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1956:77791 CAPLUS

DOCUMENT NUMBER: 50:77791

ORIGINAL REFERENCE NO.: 50:14690b-i,14691a-b

TITLE: 1,2-Cyclopentenofluorenes and some derivatives of 1,2,3-4-tetrahydrofluorene

AUTHOR(S): Bergmann, Ernst D.; Ikan, Raphael

CORPORATE SOURCE: Hebrew Univ., Jerusalem

SOURCE: Journal of the American Chemical Society (1956), 78, 2821-4
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

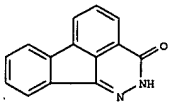
GI For diagram(s), see printed CA Issue.

AB cf. C.A. 50, 8578e. Ice water (2 l.) added to 2.5 kg. 4% Na amalgam and then with stirring during 0.5 hr. 60 g. fluorenone-1-carboxylicacid (I) (orange needles, m. 191°) while maintaining the pH of the liquid near 7 by the slow addition of HCl, the mixture heated 4 hrs. on the steam bath, cooled, filtered, and acidified with 10% H2SO4, and the precipitate recrystd. from EtOH gave 30 g. fluorene-1-carboxylicacid (II), m. 245°; the mother liquor diluted with H2O gave an addnl. 14 g. II. II (3 g.) treated at -10° with 5 g. CH2N2 in Et2O, allowed to stand 12 hrs. at room temperature, and distilled yielded 3 g. Me ester of I, b0.8 150°, m. 42°, d27 1.1250, nD27 1.5652, MRD 66.12. An attempt to reduce I by the method of Huang-Minlon gave 100% (C.A. 47, 1649a) III, colorless needles, m. 262° (from BuOAc). II (30 g.) and 180 g. SOCl2 refluxed 2 hrs. and evaporated in vacuo, the residue dissolved in C6H6 and evaporated to dryness in vacuo, and this procedure repeated several times gave 30 g. chloride (IV) of II, colorless needles, m. 108° (from C6H6). Pure H passed with stirring through 5 g. IV in 50 cc. boiling dry xylene containing 0.7 g. 10% Pd-C and 0.1 cc. Rosenmund inhibitor during 1.5 hrs., the mixture refluxed 0.5 hr., the xylene removed in vacuo, the residue distilled, and the distillate, b0.85 158°, recrystd. from cyclohexane yielded 3.5 g. fluorene-1-aldehyde (V), colorless needles, m. 72°; 2,4-dinitrophenylhydrazone, orange-red needles, m. 262° (from EtNO2). V (3 g.), 1.6 g. CH2(CO2H)2, 1.2 g. pyridine, and 3 drops piperidine heated 4 hrs. on the steam bath and 5 min. at 150°, the mixture poured into 100 cc. H2O and 5 cc. concentrated HCl, and the precipitate isolated gave 3.5 g. 3-(1-fluorenyl)acrylicacid (VI), long, colorless needles, m. 254° (from glacial AcOH). VI (3 g.) in 150 cc. dioxane hydrogenated at room temperature and 3 atmospheric pressure over 100 mg. PtO2 yielded 100% 3-(1-fluorenyl)-propionicacid (VII), colorless needles, m. 205° (from glacial AcOH). VII (2 g.) and 60 g. polyphosphoric acid heated 2 hrs. with stirring at 120-30°, poured into 200 cc. cold H2O, and extracted with Et2O, and the extract worked up gave 1.2 g. 3'-oxo-1,2-cyclopentenofluorene(VIII), yellowish needles, m. 185° (from iso-PrOH). VIII (1.3 g.), 1.4 g. KOH, 2 cc. 85% N2H4.H2O, and 10 cc. (CH2OH)2 treated by the method of Huang-Minlon (loc. cit.), diluted with 15 cc. H2O, acidified with 4 cc. 6N HCl, and extracted with CHCl3 gave 1.1 g. 1,2-cyclopentenofluorene(IX), white leaflets, m. 120° (from EtOH). MeMgI (from 0.6 g. Mg and 3.3 g. MeI) in Et2O treated with 1.7 g. solid VIII, the Et2O removed and replaced by C6H6, the mixture refluxed 4 hrs., kept 12 hrs. at room temperature, and decomposed with ice and H2SO4, and the C6H6 layer worked up gave 100% 3'-methyl-1,2-cyclopentadienofluorene (X), yellow crystals, m. 197° (from glacial AcOH). X (1 g.) in 100 cc. absolute EtOH hydrogenated at 2 atmospheric over 100 mg. PtO2 gave 100% 3'-methyl-1,2-cyclopentenofluorene, colorless crystals, m. 121° (from glacial AcOH). 1,2,3,4-Tetrahydro derivative (2 g.) of II in 100 cc. absolute EtOH hydrogenated at slightly elevated temperature over 100 mg. PtO2 yielded 1,2,3,4,1a,4a-hexahydro derivative of II, m. 138-9° (from cyclohexane). 2-Benzylcyclohexanone, b4 164-6°, m. 53-4°, cyclodehydrated with AlCl3 gave 40% 1,2,3,4-tetrahydrofluorene(XI), b6 135-40°, d27.5 1.0189, nD27.5 1.5600, MRD 54.02, silvery leaflets, m. 57° (from MeOH), and a considerable amount of resinous material; a liquid by-product, XI or an isomer, b0.4 82-4°, d25 1.0035, nD25 1.5533, MRD 54.10, was also obtained. XI (8 g.), 7 g. p-ClC6H4CHO, 1 g. piperidine, and 1 g. powdered KOH heated azeotropically in 50 cc. xylene, the solution washed with dilute acid, aqueous NaHCO3, and H2O, dried, and distilled gave some unchanged XI and then the 9-(p-chlorobenzylidene)derivativeof XI, b0.09 210-15°, beautiful lemon-yellow prisms, m. 114-15°. XI (1.65 g.) in 100 cc. absolute EtOH hydrogenated over 100 mg. PtO2 gave 1,2,3,4,1a,-4a-hexahydrofluorene, colorless oil, b0.8 98°, nD26 1.5409.

IT 36999-81-2F, Indeno[1,3-de]phthalazin-3-ol
RL: PREP (Preparation)
(preparation of)

RN 36999-81-2 CAPLUS

CN Indeno[1,2,3-de]phthalazin-3(2H)-one(7CI, 8CI, 9CI) (CA INDEX NAME)



L4 ANSWER 38 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1952:57217 CAPLUS

DOCUMENT NUMBER: 46:57217

ORIGINAL REFERENCE NO.: 46:9543d-i,9544a-b

TITLE: Ring closure of derivatives of 2-aminofluorene

AUTHOR(S): Campbell, Neil; Stafford, W. H.

CORPORATE SOURCE: Univ. Edinburgh, UK

SOURCE: Journal of the Chemical Society (1952) 299-302
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

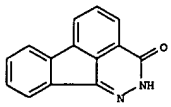
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB The product from 2-aminofluorene and (HO)2C(CO2Et)2 (Neish, C.A. 43, 193f) is Et indeno(3',2':5,6)dioxindole-3-carboxylate(I), m. 247-9° (40-50%). I (0.25 g.) in 5 mL. EtOH and 5 mL. 4 N NaOH, treated with 2 mL. 100% H2O2, warmed until O evolution ceased, diluted with 30 cc. H2O containing AcOH, and extracted with ether, gives 0.12 g. 2-amino-3-fluorenecarboxylic acid (II), m. 256°. Through the diazo compound, 0.1 g. II yields 0.042 g. 3-fluorenecarboxylic acid (III), m. 231°. Oxidation of 0.05 g. III with KMnO4 in 4 N NaOH gives 0.02 g. 9-oxo-3-fluorenecarboxylicacid (IV), yellow, m. 300-1°. I, by N.'s method, yields indeno(3',2':5,6)isatin (IVA), which was characterized by oxidation to II and by the preparation of the quinoxaline derivative, C21H13N3, yellow, m. above 350°. 9-Oxo-1-fluorenecarboxylicacid (V) (10 g.), added in portions to an emulsion of 30 g. KOH and 125 mL. Ph2O while the temperature is raised to 200°, gives a variable yield of 2-HO2CC6H4C6H4CO2H-3 (VI), m. 216-17°; Me ester, m. 71-2°. VI (2.5 g.) in 25 mL. concentrated H2SO4, heated 1 min. at 140°, gives 0.65-0.86 g. IV; the remainder is V; Me ester of VI, pale yellow, m. 145°. Mayer and Freitag (C.A. 15, 2283) isolated only 12% V. IV (0.2 g.), 5 mL. dioxane, 5 mL. AcOH, 2 mL. concentrated HCl, and a large excess of amalgamated granular Zn, boiled about 2 h. (addition of 4 portions of 1 mL. concentrated HCl), gives 0.16 g. III. 2-Amino-3-nitrofluorene, m. 203° (3 g.), yields 1.5 g. 2-bromo-3-nitrofluorene, m. 119°, by a modification of the method of Campbell, et al. (C.A. 34, 5060.8); reduction of 1.2 g. with SnCl2 in AcOH-HCl (boiled 2.5 h.) gives 0.49 g. 3-aminofluorene; work has discontinued because of the poor yield. Attempts to prepare 3-bromofluorene by the method of Miller and Bachman (C.A. 30, 1764.5) failed. The mercurichloride of M. and B. on bromination yields a dibromofluorene, m. 163°; CrO3 oxidation yields a dibromofluorenone (VII), m. 140° (2,4-dinitrophenylhydrazone, orange, m. 340°); VII with HNO3 in boiling AcOH gives a NO2 derivative, m. 192-3°. The 2nd method of M. and B. yields a (bromomercuri)dibromofluorene. The product of the Skraup reaction on 2-aminofluorene is probably indeno(3',2':6,7) quinoline (comparison of absorption spectra with those of 2,3- and 1,2-benzofluorene). V (0.2 g.) and 1 mL. 90% N2H4.H2O in 5 m. dioxane, boiled 2 h., give 0.18 g. 3-hydroxy-1,2-diazafluoranthene(C.A. numbering), m. 267-8°. V and KNO2 in H2SO4 give the 2,7-di-NO2 derivative (?), m. 267°. Fluorene, NaN3, and H2SO4 yield chiefly unchanged fluorene and a little 2,7-diaminofluorene.

IT 36999-81-2F, Indeno[1,3-de]phthalazin-3-ol

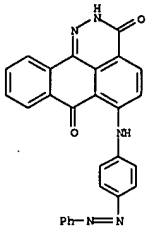
RL: PREP (Preparation)
(preparation of)
RN 36999-81-2 CAPLUS
CN Indeno[1,2,3-de]phthalazin-3(2H)-one(7CI, 8CI, 9CI) (CA INDEX NAME)



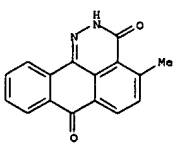
L4 ANSWER 39 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1949:45334 CAPLUS
DOCUMENT NUMBER: 43:45334
ORIGINAL REFERENCE NO.: 43:8165f-i,8166a-c
TITLE: Orange anthrapyridazone dyes for wool
INVENTOR(S): Coffey, Samuel; Schofield, Kenneth; Slinger, Frank H.; Tatum, Wm. W.
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 615837		19490112	GB 1946-24125	19460814

GI For diagram(s), see printed CA Issue.
AB Anthrapyridazone dyes (I) having the structure shown below, in which X is H or an aryl radical and R is the residue of an azobenzene, are prepared by condensing halogen derivs. of pyridazones with aminoazobenzenes and sulfonating the resulting products. The I are fast and dye wool in orange to orange-red shades. A I is prepared by condensing 6-chloro-2-phenyl-1',9'-anthrapyridaz-3-one (II) with p-aminoazobenzene (III) in the presence of KOAc and Cu bronze in PhNO2, and sulfonating the resulting 6-(p-phenylazoanilino)-2-phenyl-1',9'-pyridaz-3-one. Other I are similarly prepared by sul fonating 6-[p-(p-aminophenylazo)anilino]-2-phenyl-1',9'-anthrapyridaz-3-one (prepared by condensing II with 4,4'-diaminoazobenzene), 6-[p-(p-methoxyphenylazo)anilino]-2-phenyl-1',9'-anthrapyridaz-3-one (prepared by condensing II with 4'-methoxy-4-aminoazobenzene), 6-[p-(4-chloro-2-nitrophenylazo)anilino]-2-phenyl-1',9'-anthrapyridaz-3-one (prepared by condensing II with 4'-chloro-2'-nitro-4-aminoazobenzene), 6-p-phenylazoanilino-2-(p-nitrophenyl)-1',9'-anthrapyridaz-3-one (prepared by condensing 6-chloro-2-(p-nitrophenyl)-1',9'-anthrapyridaz-3-one (IV) with III), 6-p-phenylazoanilino-2-(2,5-dichlorophenyl)anthrapyridaz-3-one (prepared by condensing 6-chloro-2-(2,5-dichlorophenyl)-1',9'-anthrapyridaz-3-one(V) with III), or 6-p-phenylazoanilino-1',9'-anthrapyridaz-3-one (prepared by condensing 6-chloroanthrapyridazone with III. IV is prepared by heating 1-chloroanthraquinone-4-carboxylicacid (VI) and p-nitrophenylhydrazine in EtOH. V is prepared by heating VI with 2,5-dichlorophenylhydrazine in EtOH.
IT 858031-47-7, 7H-Naphtho[1,2,3-de]phthalazine-3,7-(2H)-dione, 6-(p-phenylazoanilino)-
(dye from)
RN 858031-47-7 CAPLUS
CN 7H-Naphtho[1,2,3-de]phthalazine-3,7-(2H)-dione,6-(p-phenylazoanilino)-(5CI) (CA INDEX NAME)



L4 ANSWER 40 OF 40 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1929:40448 CAPLUS
DOCUMENT NUMBER: 23:40448
ORIGINAL REFERENCE NO.: 23:4695f-i,4696a-e
TITLE: Anthrahydroquinol α-carboxylic lactones
AUTHOR(S): Scholl, Roland; Renner, Fritz; Bottger, Oskar; Hass, Sigfrid; Meyer, H. Kurt
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1929), 62B, 1278-95
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C, A. 23, 2710. In addition to the 2 methods described in the earlier papers (treatment of anthrahydroquinol α-carboxylic acids with Ac2O and of anthraquinone α-carboxylic anhydrides with Na2S2O4 alone or in the presence of dilute NH4OH or AcOH), anthrahydroquinol-1-carboxylic lactone (I) and its 2-Me derivative (II) have been prepared by the following methods: (1) Short heating of the anthraquinone acids with Zn dust and AcOH in the presence of Ac2O. (2) Reduction of the esters of the quinone acids with acid or alkaline reducing agents. The aryl esters are readily reduced by Na2S2O4 or Zn dust and NH4OH, best by Zn dust and boiling AcOH. Of the alkyl esters, only those of the 2,1-C6H4(CO)2C2H2MeCO2H (III) react in this way; those of the unmethylated C6H4(CO)2C6H3CO2H (IV) are converted exclusively into the hydroquinol acid. (3) From the acid chlorides with NaS2O4 and NaOH. (4) From the acid amides with Na2S2O4 and very dilute NaOH or AcOH. The methods involving alkalies or NH4OH are not practical as the alkaline solns. of the lactones are very unstable and sensitive to the air. The lactones, themselves red, disiolve easily in aqueous NH4OH, less readily, in NaOH and Na2CO3, with vivid pure blue color and ate reppld. red by including CO2; in the blue alkaline solns. they change more or less rapidly, by addition of H2O, into the red anthrahydroquinolcarboxylates; in the NH4OH solns. into the anthrahydroquinolcarboxamides. In C5H5N, I dissolves with its own red color and on cooling seps. from a hot concentrated solution as a red homopolar compound III.C5H5N, but if H2O is added to the red solution it becomes deep blue with formation of the heteropolar true pyrdinium salt which is dissociated back into the red form by heat or much C5H5N. The lactones are sensitive to air in alkaline, acid or neutral solution, especially in C6H6 or xylene in the light. Typical oxidizing agents (PbO2, FeCl3, K3Fe(CN)4, Br, KMnO4) oxidize them more or less rapidly at room temperature; for practical purposes hot PhNO3 is best. II in all cases gave chiefly 2,2'-dimetyl-9,9'-dihydroxy-9,9'-bianthronyl-1,1'-dicarboxylidilactone (V). The oxidation with KMnO4 in Me2CO-AcOH and with Br in C5H5N is instantaneous and quant. and may be used to titrate the lactones. V is also formed from the acid chloride of III in C6H6 with finely divided Ag or PhNMe2. Concentrated H2SO4 decomps. V. into III. Zn dust and AcOH, Na2S2O4 and NH4OH very slowly, reduce V to the monomeric II. Aqueous and especially alc. alkalies dissociate V with formation of an olive-green solution containing the salts of the anthraquinone and the anthrahydroquinol acids apparently in quinhydrone-like combination. Probably the primary process is a radical dissociation into an anthroxyl with univalent O. Exposure of V in AcOH to ultra-violet light and heating in certain organic solvents apparently also brings about a similar dissociation I, brown-red, decolorizes above 175° and begins to sublime. Ph ester of IV, m. 213°. 10-Acetate of I, from IV and Zn dust in boiling Ac2O, m. 196°. Me ester of III. light yellow, m. 178-9°; Et ester, m. 144°; Ph ester, pale yellow, m. 218-9° (2-methylpyridazonanthrone, from the Ph ester and N2H4.H2O in boiling C6H6, yellow, m. 332°); p-bromophenyl ester, yellowish, m. 226°. 2-Methylanthrahydroquinol-1-carboxylic acid is precipitated as a yellow jelly from the alkaline Na2S2O4 vat of III. The lactone (II). red, becomes lighter about 235°, m. around 265°, (decomposition). Amide of III from II allowed to stand in NH4OH and then shaken with air, or from the chloride of III in C6H6 with NH3, begins to sinter 255°, darkens 260°, decomps completely at higher temps. Acetate of II, orange, m. 238°. 2,2'-Di-Me homolog of V, turns brown on rapid heating about 270°, m. around 290° (decomposition). It had been concluded, from the work on the quinone anhydrides, that the latter have the normal structure C6H4(CO)2C5H3COR and not the ps-structure C6H4. Since in the reduction of the free quinone acid (III) to II the intermediate hydroquinol acid has been isolated and the amide is repptd. unchanged by air from its alkaline vat, it is concluded that the free anthraquinonecarboxylic acids and their amides likewise have the normal structure, and the same is shown for the esters in the following abstract
IT 858020-37-8, 7-Naphtho[1,2,3-de]phthalazine-3,7(2)-dione, 4-methyl-
RL: PREP (Preparation)
(preparation of)
RN 858020-37-8 CAPLUS
CN 7-Naphtho[1,2,3-de]phthalazine-3,7(2)-dione,4-methyl- (3CI) (CA INDEX NAME)



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FULL ESTIMATED COST	192.86	365.38

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